学位論文

Information thermodynamics on causal networks and its application to biochemical signal transduction (ネットワーク上の情報熱力学とシグナル伝達への応用)

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Abstract

We develop a general formalism of nonequilibrium thermodynamics with complex information flows (i.e., the transfer entropy) induced by interactions among multiple fluctuating systems. Characterizing nonequilibirium dynamics by causal networks (i.e., Bayesian networks), we obtain novel generalizations of the second law of thermodynamics and the fluctuation theorem, which include an informational quantity given by the topology of the networks. Our formalism on causal networks gives thermodynamics for small subsystems as a generalization of the stochastic thermodynamics with information. Our theory is called "information thermodynamics on causal networks".

Information thermodynamics on causal networks is applicable to quite a broad class of nonequilibrium stochastic dynamics such as information transfer between multiple Brownian particles, an autonomous biochemical reaction described by the master equation, and complex dynamics in multiple fluctuating systems. Our result can produce the previous study of the Maxwell's demon for a special case of the feedback control with a single measurement.

As an application of our general formalism, we can discuss the accuracy of the information transmission in the biochemical signal transduction of sensory adaptation, where there is not any explicit channel coding in contrast to the case of Shannon's information theory. Focusing on the robustness of the signal transduction against the environmental noise, we show the analogical similarity between our information thermodynamic result and Shannon's noisy-channel coding theorem. Our result can open up a novel biophysical and thermodynamic approach to understand information processing in living system.

In our study, we clarify the physical meaning of information flow from a thermodynamic point of view. Information flow given by the transfer entropy from the target system to the outside worlds characterizes the thermodynamic benefit of the target system under the condition of the outside worlds. We also propose the novel information flow called the "backward" transfer entropy, which characterizes the inevitable thermodynamic dissipation of the target system because of the effects of outside worlds.

By the above, information thermodynamics on causal networks will be a basis of the statistical physics and biophysics from the viewpoint of the information flow.

Contents

Chapter 1

Introduction

After the publication of Shannon's influential paper about an artificial communication [1], the importance of information theory has been increasing and several fields of informational study has been emerging [2, 3]. Our study in this thesis is a challenge for developing a novel field of physics with information, so-called information thermodynamics as a fundamental theory of nonequilibrium physics including biophysics.

Nowadays, we can see information device such as a computer everywhere. On the basis of Shannon's information theory, the information quantity such as the mutual information gives the coding redundancy and the accuracy of information transmission in artificial channel coding [1, 2]. From the viewpoint of the artificial information transmission, the classical information theory has been well established, and we can quantitatively discuss the efficiency of coding and the accuracy of information transmission using the entropic quantities. The classical theory of communication (i.e., the noisy-channel coding theorem) is completely based on the assumption of the existence of artificial coding devices (i.e., the encoder and the decoder). Without artificial channel coding, the physical meaning of informational quantity is elusive in terms of the accuracy of signal transmission. The non-existence of channel coding is crucial in living systems. For example, the biochemical signal transduction network inside or outside cells is an example of nonequilibrium fluctuating dynamics, which describes information transmission without artificial coding devices [4, 5]. Many researchers intuitively believe the importance of information flow in biochemical system to maintain life, and several studies have tried out to reveal the role of the information transfer on biochemical networks. For example, the informational quantity such as the mutual information in the biochemical signal transduction has been calculated theoretically [6], and measured experimentally for several biochemical systems [7, 8, 9, 10, 11]. However, due to the lack of the fundamental information theory for the biological system without the explicit artificial channel coding, the application of the information theory to the biological system has been unclear. Thus, the physical meaning of the mutual information inside the biochemical system can be just a measure of independence between two fluctuating components by definition. Although we usually say "information" in a natural sense of the biochemical signal transduction, we do not have a fundamental theory of information for living systems like the noisy-channel coding theorem for artificial communication. To discuss the physical meaning of "information" in living systems, we believe that we need more physical and fundamental theory of information transmission in nonequilibrium dynamics instead of the conventional information theory.

On the other hand, the study of thermodynamics [12, 13, 14, 15] for a stochastic nonequilibrium system (e.g., a Brownian particle, bio-polymer, enzyme, and molecular motor) with information has been intensively discussed recently [16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66], in relation to the study of Maxwell's demon which is the thought experiment about the validity of thermodynamics for a small systems in the19th century [13, 67, 68]. Before Shannon established the classical information theory, Leo Szilard had discussed the minimal model of Maxwell's demon, and show the relationship between the "Shannon" entropy and thermodynamics in 1929 [69]. In the last two decades, nonequilibrium equalities that are universally valid for a nonequilibrium small system, have been found [70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87], and experimentally verified for several systems including the biopolymer and the molecular motor [88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98]. Based on the backgrounds of nonequilibrium equalities, thermodynamics under the feedback control has been established by considering Maxwell's demon as a feedback controller [25] and experimentally verified [64, 65, 66] as a refinement of the discussion by Leo Szilard. While the relationship between information and thermodynamics has been studied in several simple setups with the demon [26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49], the general theory that can be applied to the complex situations, such as biochemical signal transduction, had been elusive before publishing our results [50, 59].

In this thesis, we develop the general formalism of nonequilibrium dynamics on causal networks, by using the information theory and nonequilibrium statistical physics [50, 59]. We mainly discuss the following two questions:

- Beyond the simple setup of Maxwell's demon, how do we develop the theory of stochastic thermodynamics with information that should be generally valid for complex nonequilibrium dynamics?
- What is the physical meaning of information flow in biochemical signal transduction, to which we cannot explicitly apply the noisy-channel coding theorem?

As a generalization of the study of Maxwell's demon, we propose a general formalism of the study of nonequilibrium thermodynamics with complex information flows induced by interactions between multiple fluctuating systems [50]. Characterizing the complex dynamics by the causal networks (i.e., the Bayesian networks) which can represent quite a broad class of nonequilibrium dynamics such as multiple Brownian particles and complex structure of the biochemical signal transduction [99, 100, 101, 102, 103, 104], we obtain a novel generalization of the second law of thermodynamics with complex information flows. In our generalization of the second law, the transfer entropy [105], which is a measure of the causal relationship and information flow [106, 107, 108, 109], plays a crucial role as a lower bound of the entropy production in a small subsystem.

Our study can be regarded as a general graphical formalism of thermodynamics with information flow so-called "information thermodynamics on causal networks", which gives thermodynamics for a small subsystem described by the causal networks. Focusing on information flow characterizing the topology of the causal networks, we show the fact that thermodynamical entropy production in a partial target system is generally bounded by the information flow (i.e., the transfer entropy) from the target system to outside worlds. In the generalization of the second law of thermodynamics, we propose a novel information quantity called "backward" transfer entropy [50], as an inevitable loss of thermodynamical benefit by information flow.

We apply our general result to a simple biochemical signal transduction of *E. coli* bacterial chemotaxis [50], as a simple examination of the signal transmission in nonequilibrium biochemical system. We find that our information thermodynamics performs as a biochemical theory of communication without artificial channel coding device. We generally show that the robustness of biochemical signal transduction against the environmental noise is bounded by the conditional mutual information between input and output. While it is remarkable that this information thermodynamic argument is very similar to the argument of Shannon's noisy-channel coding theorem, there is a crucial difference between information thermodynamics and the noisy-channel coding theorem. In the biological signal transduction, it is impossible to define the archivable rate as the accuracy of signal transduction in the sense of the noisy-channel coding theorem, because the signal transduction is achieved by a coupled chemical reaction and there exists no artificial encoding or decoding device that produces a redundant bit sequence. In contrast, the thermodynamic definition of the robustness of the signal transduction proposed in our study is intrinsically related to the dynamics of the biochemical signal transduction, and therefore powerful to characterize its robustness. Our result can be experimentally validated by measuring the amount of proteins during signal transduction in the same way as in the previous experiments [8, 9, 10, 11], and we can discuss the thermodynamic efficiency of the information transmission inside cells without explicit coding device.

We organize this thesis as follows [see also Figure 1.1]. The review parts are in Chapters 2, 3, 4, and 5. The main results of this thesis are in Chapters 6, 7, 8, and 9.

In Chapter 2, we review the basis of the classical information theory well established by Shannon. We introduce the informational quantities (i.e., the Shannon entropy, the relative entropy, the mutual information and the transfer entropy), which play a crucial role in this thesis. We discuss the argument of the classical information transmission through a noisy communicational channel by Shannon (i.e., the noisy-channel coding theorem), for comparison with our main result of biochemical signal transduction in Chapter 7.

In Chapter 3, we summarize the modern thermodynamic theory for small classical systems called the stochastic thermodynamics [72, 73, 74]. We review stochastic thermodynamics in terms of the relative entropy. We derive the second law of thermodynamics from the nonnegativity of the relative entropy. We discuss two applications of stochastic thermodynamics (i.e., the steady-state thermodynamics [113, 114, 115] and feedback cooling [116, 31, 39, 169, 117, 118, 119, 120, 121]).

In Chapter 4, we focus on the relationship between stochastic thermodynamics and information theory. In particular, we review the study of Maxwell's demon, which is the second law of thermodynamics under the feedback control (i.e., the Sagawa-Ueda

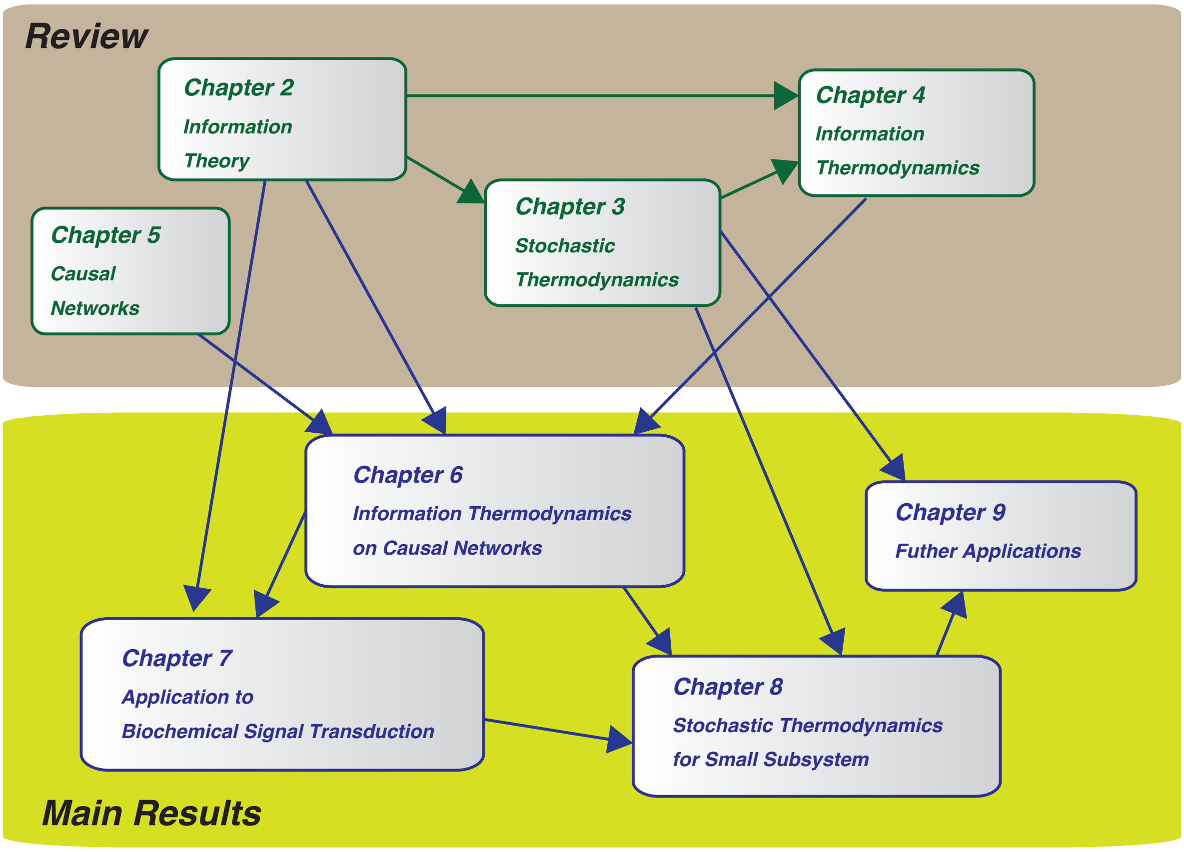

Fig. 1.1 The network of this thesis. Each chapter has such a cause-effect relationship, which is described by directed edges ($\rightarrow$) between nodes (i.e., Chapters 2-9). In our thesis, such a network plays a crucial role to discuss stochastic thermodynamics with information flow.

relation [25, 43]). In the case of feedback control, the mutual information gives a bound of an apparent violation of the second law. We discuss the minimal model of Maxwell's demon (i.e., Szilard engine [69]) as an example of the trade off between information and thermodynamic entropy.

In Chapter 5, we introduce the probabilistic graphical model well known as the Bayesian networks or causal networks [99, 100, 102, 104], which is a basis of our main study in this thesis. We introduce the mathematical definition of the causal networks, and show how to use causal networks for several physical situations.

Chapter 6 is the main part of this thesis. Characterizing complex nonequilibrium dynamics by causal networks, we construct a general formalism of the information thermodynamics and derive the generalized second law of thermodynamics with information flow. On causal networks, we show the fact that the entropy production of the target system is generally bounded by the informational quantity, which includes the mutual information of the initial correlation between the target system and outside worlds, the mutual information of the final correlation between them, and the the transfer entropy from the target system to outside worlds during the dynamics. Our result can be a novel law of thermodynamics with information flow for classical small subsystems.

In Chapter 7, we apply our main result to the biochemical signal transduction of the sensory adaptation and discuss the accuracy of the signal transmission in biological systems, where any explicit channel coding device does not exist in contrast to the noisy-channel coding theorem in Chapter 2. We find the analogical similarity between our information thermodynamic result and Shannon's noisy-channel coding theorem. We believe that our information thermodynamic approach is more relevant and measurable in biochemical systems than Shannon's noisy-channel coding theorem. We analytically and numerically show that the signal transduction model of *E. coli* chemotaxis is highly dissipative as a thermodynamic engine, but efficient as an information transmission device.

In Chapter 8, we discuss further generalizations of our main result in Chapter 6. First we focus on information thermodynamics for a multi-dimensional Markov process, and show the several relationship of information thermodynamics. We also derive another expression of our main result using the Fokker-Planck equation [122]. From this expression, our result can be interpreted as the stochastic thermodynamics for small subsystem. Next, we discuss the importance of the "backward" transfer entropy, which is the novel information quantity that we introduced in Chapters 6 and 7. From the data processing inequality [2], we derive that the bound involving the backward transfer entropy is tighter than the informational quantity discussed in Chapter 6, as a lower bound of the entropy production.

In Chapter 9, we generalize our main result for the steady-state thermodynamics introduced in Chapter 3. We also apply our main result to the feedback cooling. We show that the transfer entropy gives a lower bound of the kinetic temperature, and discuss the relationship between our main result and the third law of thermodynamics [123], as the refinement of our previous study [31].

In Chapter 10, we conclude this thesis and discuss our future prospect.

Chapter 2

Review of Classical Information Theory

We review the classical information theory in this chapter. The classical information theory had been well established by Shannon in his historical paper entitled "A mathematical theory of communication" [1]. Shannon discussed the relationship between the entropy and the accuracy of the information transmission through a noisy communication channel with an artificial coding device, which is well known as the noisy channel coding theory. In this chapter, we introduce various types of the entropy (i.e. the Shannon entropy, the relative entropy, the mutual information and the transfer entropy [105]) as measures of information, and the noisy channel coding theorem [1, 2, 124].

2.1 Entropy

First of all, we briefly introduce various types of the entropy, which quantify measures of information [1, 2].

2.1.1 Shannon Entropy

We first introduce the Shannon entropy, which characterizes the uncertainty of random variables. Let $p(x)$ be the probability distribution of a discrete random variable x. The probability distribution $p(x)$ satisfies the normalization of the probability and the nonnegativity (i.e., $\sum_x p(x) = 1$, $0 \leq p(x) \leq 1$). The Shannon entropy $S(x)$ is defined as

$$S(x) := -\sum_x p(x) \ln p(x). \tag{2.1}$$

In the case of a continuous random variable x with probability density function $p(x)$ which satisfies the normalization and the nonnegativity (i.e., $\int dxp(x) = 1$, $0 \leq p(x) \leq 1$), the Shannon entropy (or differential entropy) is defined as

$$S(x) := -\int dxp(x) \ln p(x). \tag{2.2}$$

In this thesis, the logarithm (ln) denotes the natural logarithm. To discuss the discrete and continuous cases in parallel, we introduce the ensemble average $\langle f(x) \rangle$ for any function $f(x)$ as

$$\langle f(x) \rangle = \langle f(x) \rangle_p \tag{2.3}$$
$$:= \sum_x p(x) f(x) \tag{2.4}$$

for a discrete random variable x and

$$\langle f(x) \rangle = \langle f(x) \rangle_p \tag{2.5}$$
$$:= \int dx p(x) f(x) \tag{2.6}$$

for a continuous random variable x. From the definition of ensemble average Eqs. (2.4) and (2.6), the two definitions of the Shannon entropy Eqs. (2.1) and (2.2) are rewritten as

$$S(x) = \langle - \ln p(x) \rangle \tag{2.7}$$
$$= \langle s(x) \rangle, \tag{2.8}$$

where we here say $s(x) := - \ln p(x)$ is a stochastic Shannon entropy. The Shannon entropy $S(X)$ of a set of random variables $X = \{x_1, \ldots, x_N\}$ with a joint probability distribution $p(X)$ is also defined as

$$S(X) := \langle - \ln p(X) \rangle \tag{2.9}$$
$$= \langle s(X) \rangle. \tag{2.10}$$

Let the conditional probability distribution of X under the condition Y be $p(X|Y) := p(X,Y)/p(Y)$. The conditional Shannon entropy $S(X|Y)$ with a joint probability $p(X)$ is defined as

$$S(X|Y) := \langle - \ln p(X|Y) \rangle \tag{2.11}$$
$$= \langle s(X|Y) \rangle, \tag{2.12}$$

where $s(X|Y) := - \ln p(X|Y)$ is a stochastic conditional Shannon entropy. We note that its ensemble takes an integral over a joint distribution $p(X)$. From $0 \leq p \leq 1$, the Shannon entropy S satisfies the nonnegativity $S \geq 0$.

By the definition of the conditional probability distribution $p(X|Y) := p(X,Y)/p(Y)$, we have the chain rule in probability theory. The chain rule in probability theory produces the product of conditional probabilities:

$$p(X) = p(x_1) \prod_{k=2}^{N} p(x_k | x_{k-1}, \ldots, x_1). \tag{2.13}$$

From this chain rule Eq. (2.13) and the definitions of the Shannon entropy Eqs. (2.10) and (2.12), we obtain the chain rule for (stochastic) Shannon entropy:

$$s(X) = s(x_1) + \sum_{k=2}^{N} s(x_k|x_{k-1}, \dots, x_1). \tag{2.14}$$

$$S(X) = S(x_1) + \sum_{k=2}^{N} S(x_k|x_{k-1}, \dots, x_1). \tag{2.15}$$

The chain rule indicates that the (stochastic) joint Shannon entropy is always rewritten by a sum of the (stochastic) conditional Shannon entropy.

2.1.2 Relative Entropy

We next introduce the relative entropy (or the Kullback-Leibler divergence), which is an asymmetric measure of the difference between two probability distributions. The thermodynamic relationships (e.g., the second law of thermodynamics) and several theorems in information theory can be derived from the nonnegativity of the relative entropy. The relative entropy or the Kullback-Leibler divergence between two probability distributions $p(x)$ and $q(x)$ is defined as

$$D_{\mathrm{KL}}(p(x)||q(x)) = \langle \ln p(x) - \ln q(x) \rangle_p. \tag{2.16}$$

We will show that the relative entropy is always nonnegative and is 0 if and only if $p = q$.

To show this fact, we introduce Jensen's inequality [2]. Let $\phi(f(x))$ be a convex function, which satisfies $\phi(\lambda a + (1-\lambda)b) \leq \lambda\phi(a) + (1-\lambda)\phi(b)$ with $\forall a, b \in f(x)$ and $\forall \lambda \in [0, 1]$. Jensen's inequality states

$$\phi(\langle f(x) \rangle) \leq \langle \phi(f(x)) \rangle. \tag{2.17}$$

The equality holds if and only if $f(x)$ is constant or ϕ is linear.

We notice that $-\ln(f(x))$ is a convex nonlinear function. By applying Jensen's inequality (2.17), we can derive the nonnegativity of the relative entropy,

$$\begin{aligned} D_{\mathrm{KL}}(p(x)||q(x)) &= \langle -\ln[q(x)/p(x)] \rangle_p & (2.18)\\ &\geq -\ln \langle q(x)/p(x) \rangle_p & (2.19)\\ &= -\ln 1 & (2.20)\\ &= 0, & (2.21)\end{aligned}$$

where we used the normalization of the distribution q, $\langle q(x)/p(x) \rangle_p = \int dx q(x) = 1$. The equality holds if and only if $q(x)/p(x) = c$, where c is a constant. Because p and q satisfy the normalizations $\int dx p(x) = 1$ and $\int dx q(x) = 1$, a constant c should be $c = 1$, and we can show that the relative entropy $D_{\mathrm{KL}}(p(x)||q(x))$ is 0 if and only if $p = q$.

From the nonnegativity of the relative entropy, we can easily show that $S(x) \leq \ln |x|$ where $|x|$ denotes the number of elements of a discrete random variable x with the equality satisfied if and only if x is uniformly distributed. Let $p_u(x) = 1/|x|$ be a uniform function over x. The relative entropy $D_{\mathrm{KL}}(p(x)||p_u(x))$ is calculated as $D_{\mathrm{KL}}(p(x)||p_u(x)) = \ln |x| - S(x)$, and its negativity gives $S(x) \leq \ln |x|$.

The joint relative entropy $D_{\mathrm{KL}}(p(X)||q(X))$ is defined as

$$D_{\mathrm{KL}}(p(X)||q(X)) = \langle \ln p(X) - \ln q(X) \rangle_p \tag{2.22}$$

and the conditional relative entropy $D_{\mathrm{KL}}(p(X|Y)||q(X|Y))$ is defined as

$$D_{\mathrm{KL}}(p(X|Y)||q(X|Y)) = \langle \ln p(X|Y) - \ln q(X|Y) \rangle_p. \tag{2.23}$$

The joint and conditional relative entropy satisfy $D_{\mathrm{KL}} \geq 0$ with the equality satisfied if and only if $p = q$. The chain rule in probability theory Eq. (2.13) and the definition of the relative entropy Eqs. (2.23) and (2.22) give the chain rule for relative entropy as

$$\begin{aligned} &D_{\mathrm{KL}}(p(X)||q(X)) \\ &= D_{\mathrm{KL}}(p(x_1)||q(x_1)) + \sum_{k=2}^{N} D_{\mathrm{KL}}(p(x_k|x_{k-1},\ldots,x_1)||q(x_k|x_{k-1},\ldots,x_1)). \end{aligned} \tag{2.24}$$

2.1.3 Mutual Information

We introduce the mutual information I, which characterizes the correlation between random variables. The mutual information between X and Y is given by the relative entropy between the joint distribution $p(X,Y)$ and the product distribution $p(X)p(Y)$:

$$\begin{aligned} I(X:Y) &:= D_{\mathrm{KL}}(p(X,Y)||p(X)p(Y)) \\ &= \langle \ln p(X,Y) - \ln p(X) - \ln p(Y) \rangle \\ &= \langle s(X) + s(Y) - s(X,Y) \rangle \\ &= S(X) + S(Y) - S(X,Y) \\ &= S(X) - S(X|Y) \\ &= S(Y) - S(Y|X). \end{aligned} \tag{2.25}$$

The mutual information quantifies the amount of information in X about Y (or information in Y about X). From the nonnegativity of the relative entropy $D_{\mathrm{KL}} \geq 0$, the mutual information is nonnegative $I(X:Y) \geq 0$ with the equality satisfied if and only if X and Y are independent $p(X,Y) = p(X)p(Y)$. This nonnegativity implies the fact that conditioning reduces the Shannon entropy (i.e., $S(X|Y) \leq S(X)$). From the nonnegativity of the Shannon entropy $S \geq 0$, the mutual information is bounded by the Shannon entropy of each variable X or Y ($I(X:Y) \leq S(X)$ and $I(X:Y) \leq S(Y)$). To summarize the nature of the mutual information, the following Venn's diagram is useful (see Figure 2.1).

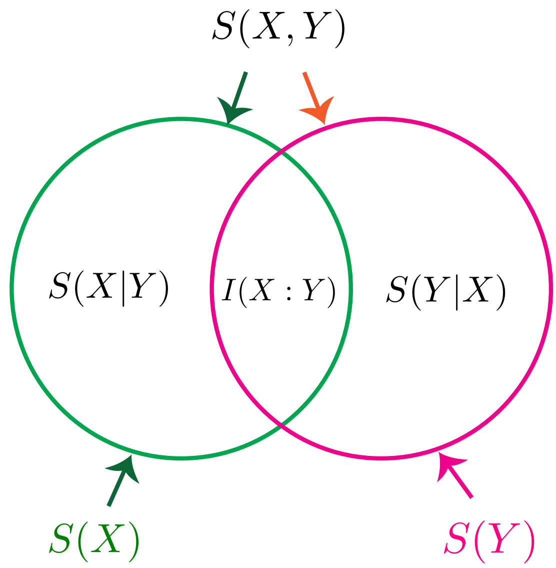

Fig. 2.1 The Venn's diagram which represents the nature of the mutual information (i.e., Eq. 2.25). The mutual information between X and Y represents the correlation between them in the sense of the Shannon entropy.

The conditional mutual information between X and Y under the condition Z is also defined as

$$\begin{aligned} I(X:Y|Z) &:= D_{\mathrm{KL}}(p(X,Y|Z)||p(X|Z)p(Y|Z)) \\ &= \langle \ln p(X,Y|Z) - \ln p(X|Z) - \ln p(Y|Z) \rangle \\ &= \langle s(X|Z) + s(Y|Z) - s(X,Y|Z) \rangle \\ &= S(X|Z) + S(Y|Z) - S(X,Y|Z) \\ &= S(X|Z) - S(X|Y,Z) \\ &= S(Y|Z) - S(Y|X,Z). \end{aligned} \tag{2.26}$$

For Z independent of X and Y (i.e., $p(X,Y|Z) = p(X,Y)$), we have $I(X:Y|Z) = I(X:Y)$. The conditional mutual information is also nonnegative $I(X:Y|Z) \geq 0$ with the equality satisfied if and only if X and Y are independent under the condition of Z: $p(X,Y|Z) = p(X|Z)p(Y|Z)$ (or $p(X|Y,Z) = p(X|Z)$). We also define the stochastic mutual information $i(X:Y)$ and the stochastic conditional mutual information $i(X:Y|Z)$ as

$$i(X:Y) := s(X|Z) + s(Y|Z) - s(X,Y|Z) \tag{2.27}$$

$$i(X:Y|Z) := s(X|Z) + s(Y|Z) - s(X,Y|Z) \tag{2.28}$$

From the chain rule for (stochastic) Shannon entropy Eq. (2.15) and the definition of the mutual information Eqs. (2.25) and (2.26), we have the chain rule for (stochastic) mutual information

$$i(X:Y) := i(x_1:Y) + \sum_{k=2}^{N} i(x_k:Y|x_{k-1},\dots,x_1), \tag{2.29}$$

$$I(X:Y) := I(x_1:Y) + \sum_{k=2}^{N} I(x_k:Y|x_{k-1},\dots,x_1). \tag{2.30}$$

2.1.4 Transfer Entropy

Here, we introduce the transfer entropy, which characterizes the directed information flow between two systems in evolving time $X = \{x_k|k = 1,\dots,N\}$ and $Y = \{y_k|k = 1,\dots,N\}$. The transfer entropy was ordinarily introduced by Schreiber in 2000 [105] as a measure of the causal relationship between two random time series. The transfer entropy from X to Y at time k is defined as the conditional mutual information:

$$\begin{aligned} \mathcal{T}_{X\to Y} &:= I(y_{k+1}:\{x_k,\dots,x_{k-l}\}|y_k,\dots,y_{k-l'}) && (2.31)\\ &= \langle s(y_{k+1}|x_k,\dots,x_{k-l},y_k,\dots,y_{k-l'}) - s(y_{k+1}|y_k,\dots,y_{k-l'})\rangle && (2.32)\\ &= \langle \ln p(y_{k+1}|y_k,\dots,y_{k-l'}) - \ln p(y_{k+1}|x_k,\dots,x_{k-l},y_k,\dots,y_{k-l'})\rangle. && (2.33)\end{aligned}$$

The indexes l and l' denote the lengths of two causal time sequences $\{x_k,\dots,x_{k-l}\}$ and $\{y_{k+1},y_k,\dots,y_{k-l'}\}$. Because of the nonnegativity of the mutual information $I(y_{k+1}:\{x_k,\dots,x_{k-l}\}|y_k,\dots,y_{k-l'})$, the transfer entropy is always nonnegative and is 0 if and only if the time evolution of Y system at time k does not depend on the history of X system,

$$p(y_{k+1}|y_k,\dots,y_{k-l'}) = p(y_{k+1}|x_k,\dots,x_{k-l},y_k,\dots,y_{k-l'}). \tag{2.34}$$

Thus, the transfer entropy quantifies the causal dependence between them at time k. If the dynamics of X and Y is Markovian (i.e., $p(y_{k+1}|x_k,\dots,x_{k-l},y_k,\dots,y_{k-l'}) = p(y_{k+1}|x_k,y_k)$), the most natural choices of l and l' becomes $l = l' = 0$ in the sense of the causal dependence.

Here, we compare other entropic quantities which represent the direction exchange of information. Such conditional mutual informations have been discussed in the context of the causal coding with feedback [127]. Massey defined the sum of the conditional mutual information

$$I^{\mathrm{DI}}(X\to Y) := \sum_{k=1}^{N} I(y_k:\{x_1,\dots,x_k\}|y_{k-1},\dots,y_1), \tag{2.35}$$

called the directed information. It can be interpreted as a slight modification of the sum of the transfer entropy over time. Several authors [125, 126] have also introduced the mutual information with time delay to investigate spatiotemporal chaos.

In recent years, the transfer entropy has been investigated in several contexts. For a Gaussian process, the transfer entropy is equivalent to the Granger causality test [106], which is an economic statistical hypothesis test for detecting whether one time series is useful in forecasting another [107, 108]. Using a technique of symbolization, a fast and robust calculation method of the transfer entropy has been proposed [109]. In a study of the order-disorder phase transition, the usage of the transfer entropy has been also proposed to predict an imminent transition [128]. In relation to our study, thermodynamic interpretations of the transfer entropy [129, 130] and a generalization of the transfer entropy for causal networks [131] have been proposed.

2.2 Noisy-Channel Coding Theorem

In this section, we show the fact that the mutual information between input and output is related to the accuracy of signal transmission. This fact is well known as the noisy-channel coding theorem (or Shannon's theorem) [1, 2]. The noisy-channel coding theorem was proved by Shannon in his original paper in 1948 [1]. In the case of Gaussian channel, a similar discussion of information transmission was also given by Hartley previously [124].

2.2.1 Communication Channel

We consider the noisy communication channel. Let x be the input of the signal and y be the output of the signal. The mutual information $I(x : y)$ represents the correlation between input and output, which quantifies the ability of information transmission through the noisy communication channel. Here, we introduce two simple examples of the mutual information of the communication channel.

2.2.1.1 Example 1: Binary symmetric channel

Suppose that the input and output are binary states $x = 0, 1$ and $y = 0, 1$. The noise in the communication channel is represented by the conditional probability $p(y|x)$. The binary symmetric channel is given by the following conditional probability,

$$p(y = 1|x = 1) = p(y = 0|x = 0) = 1 - e, \tag{2.36}$$

$$p(y = 1|x = 0) = p(y = 1|x = 1) = e, \tag{2.37}$$

where e denotes the error rate of the communication. We assume that the distribution of the input signal is given by $p(x = 1) = 1 - r$ and $p(x = 0) = r$. The mutual information between input and output is calculated as

$$I(x : y) =(1 - e) \ln(1 - e) + e \ln e - (1 - e') \ln(1 - e') - e' \ln e', \tag{2.38}$$

where $e' := (1 - e)r + e(1 - r)$. This mutual information represents the amount of information transmitted through the noisy communication channel. In the case of $e = 1/2$, we have $I(x : y) = 0$, which means that we cannot infer the input signal x from reading the output y. The mutual information depends on the bias of the input signal r. To discuss the nature of the communication channel, the supremum value of the mutual information between input and output with respect to the input distribution. Let the channel capacity for the discrete input be

$$C := \sup_{p(x)} I(x : y). \tag{2.39}$$

For a binary symmetric channel, the mutual information has a supremum value with $r = 1/2$, and the channel capacity C is given as

$$C = \ln 2 + e \ln e + (1 - e) \ln(1 - e). \tag{2.40}$$

2.2.1.2 Example 2: Gaussian channel

Suppose that the input and output have continuous values: $x \in [-\infty, \infty]$ and $y \in [-\infty, \infty]$. The Gaussian channel is given by the Gaussian distribution:

$$p(y|x) = \frac{1}{\sqrt{2\pi\sigma_N^2}} \exp\left[-\frac{(x-y)^2}{2\sigma_N^2}\right], \tag{2.41}$$

where σ_N^2 denotes the intensity of the noise in the communication channel. We assume that the initial distribution is also Gaussian:

$$p_P(x) = \frac{1}{\sqrt{2\pi\sigma_P^2}} \exp\left[-\frac{x^2}{2\sigma_P^2}\right], \tag{2.42}$$

where $\sigma_P^2 = \langle x^2 \rangle$ means the power of input signal. The mutual information $I(x : y)$ is calculated as

$$I(x : y) = \frac{1}{2} \ln\left(1 + \frac{\sigma_P^2}{\sigma_N^2}\right). \tag{2.43}$$

In the limit $\sigma_N^2 \to \infty$, we have $I(x : y) \to 0$, which indicates that any information of input signal x cannot be obtained from output y if the noise in communication channel is extremely large. We have $I(x : y) \to \infty$ in the limit $\sigma_P^2 \to \infty$, which means that the power of input is needed to send much information.

In the continuous case, the definition of the channel capacity is modified with the power constraint:

$$C = \sup_{\langle x^2 \rangle \le \sigma_P^2} I(x : y). \tag{2.44}$$

The channel capacity C is given by the mutual information with the initial Gaussian distribution Eq. (2.43),

$$C = \frac{1}{2} \ln\left(1 + \frac{\sigma_P^2}{\sigma_N^2}\right). \tag{2.45}$$

To show this fact, we prove that the mutual information $I_q(x : y) = \langle \ln p(y|x) - \ln \int dx p(y|x) q(x) \rangle$ for any initial distribution $q(x)$ with $\langle x^2 \rangle = \sigma_{P'}^2 \le \sigma_P^2$ is always lower than the mutual information for a Gaussian initial distribution Eq. (2.43).

$$\begin{aligned}
I(x : y) - I_q(x : y) &= -\langle \ln p_P(y) \rangle_{p_P} + \langle \ln q(y) \rangle_q && (2.46)\\
&\ge -\langle \ln p_{P'}(y) \rangle_{p_{P'}} + \langle \ln q(y) \rangle_q && (2.47)\\
&= -\langle \ln p_{P'}(y) \rangle_q + \langle \ln q(y) \rangle_q && (2.48)\\
&= D_{\mathrm{KL}}(q(y) || p_{P'}(y)) && (2.49)\\
&\ge 0, && (2.50)
\end{aligned}$$

where $p_P(x,y) := p(y|x)p_P(x)$, $q(x,y) := p(y|x)q(x)$, and we use $\langle -\ln p_P(y)\rangle_{p_P} = 2^{-1}\ln[2\pi(\sigma_P^2+\sigma_N^2)] + 2^{-1}$.

2.2.2 Noisy-Channel Coding Theorem

We next review the noisy-channel coding theorem, which is the basic theorem of information theory stated by Shannon in his original paper [1].

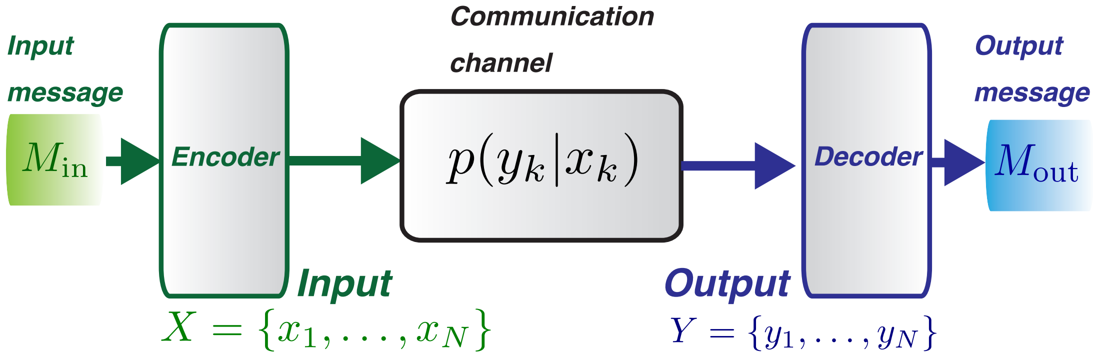

Fig. 2.2 Schematic of the communication system. To send an input message M_{in} through a noisy artificial communication channel, the input message should be encoded in a redundant sequence of bits by a channel coding protocol, and the encoded bits sequence X is transmitted through a noisy communication channel $p(y_k|x_k)$ (e.g., a Gaussian channel). The output sequence Y does not necessary coincide with the input sequence X, because of the noise in the communication channel. However, if the redundancy N of the encoded bit sequence is sufficiently large, one can recover the original input message $M_{\mathrm{out}} = M_{\mathrm{in}}$ correctly from the output sequence Y. This is a sketch of the channel coding.

Here, we consider the situation of information transmission through a noisy communication channel (see also Figure 2.2). First, the input message is encoded to generate a sequence of the signal (e.g. 0010101010). Second, this signal is transmitted through a noisy communication channel. Finally, the output signal (e.g. 0011101011) is decoded to generate the output message.

To archive the exact information transmission through a noisy communication channel, the length of encoding should be sufficiently large to correct the error in output signal. The noisy-channel coding theorem states the relationship between the length of encoding (i.e., the archivable rate) and the noise in the communication channel (i.e., the channel capacity). Strictly speaking, the noisy-channel coding theorem contains two statements, the noisy-channel coding theorem and the converse to the noisy-channel coding theorem. The former states the existence of coding, and the latter states an upper bound of the coding length. In this section, we introduce the noisy-channel coding theorem for a simple setting.

Let the input message be $M_{\mathrm{in}} \in \{1, \ldots, M\}$, where M denotes the number of types of the message. The input message is assumed to be uniformly distributed: $p(M_{\mathrm{in}}) = 1/M$ $(M_{\mathrm{in}} = 1, \ldots, M)$. By the encoder, the input message is encoded as a discrete sequence $X(M_{\mathrm{in}}) := \{x_1(M_{\mathrm{in}}), \ldots, x_N(M_{\mathrm{in}})\}$. Through a noisy communication channel defined as the conditional probability $p(y_k|x_k)$ (e.g., the binary symmetric channel), the output signal $Y = \{y_1, \dots, y_N\}$ is stochastically obtained from the input signal X:

$$p(Y|X(M_{\mathrm{in}})) = \prod_{k=1}^{N} p(y_k|x_k(M_{\mathrm{in}})), \tag{2.51}$$

which represents a discrete memoryless channel. The output message $M_{\mathrm{out}}(Y)$ is a function of the output signal Y. We define the rate as

$$R := \frac{\ln M}{N}, \tag{2.52}$$

which represents the encoding length N to describe the number of the input messages M. A code (M, N) indicates (i) an index set $\{1, \dots, M\}$, (ii) an encoding function $X(M_{\mathrm{in}})$ and (iii) a decoding function $M_{\mathrm{out}}(Y)$. A code (e^{NR}, N) means $(\lceil e^{NR} \rceil, N)$, where $\lceil \dots \rceil$ denotes the ceiling function. Let the arithmetic average probability of error P_e for a code (e^{NR}, N) be

$$P_e := \frac{1}{M} \sum_{j}^{M} p(M_{\mathrm{out}}(Y) \neq j | X(M_{\mathrm{in}} = j)). \tag{2.53}$$

In this setting, we have the noisy-channel coding theorem.

Theorem *(Noisy-channel coding theorem)* *(i) For every rate $R < C$, there exists a code (e^{NR}, N) with $P_e \to 0$.*

(ii) Conversely, any code (e^{NR}, N) with $P_e \to 0$ must have $R \leq C$.

The converse theorem (ii) can be easily proved using the nonnegativity of the relative entropy. Here, we show the proof of the converse theorem. From the initial distribution $p(M_{\mathrm{in}})$, we have

$$NR = S(M_{\mathrm{in}}) \tag{2.54}$$
$$= I(M_{\mathrm{in}} : M_{\mathrm{out}}) + S(M_{\mathrm{in}}|M_{\mathrm{out}}). \tag{2.55}$$

We introduce a binary state E: $E := 0$ for $M_{\mathrm{in}} = M_{\mathrm{out}}$ and $E := 1$ for $M_{\mathrm{in}} \neq M_{\mathrm{out}}$. From $S(E|M_{\mathrm{in}}, M_{\mathrm{out}}) = 0$, we have

$$\begin{aligned} S(M_{\mathrm{in}}|M_{\mathrm{out}}) &= S(M_{\mathrm{in}}|M_{\mathrm{out}}) + S(E|M_{\mathrm{in}}, M_{\mathrm{out}}) \\ &= S(E|M_{\mathrm{out}}) + S(M_{\mathrm{in}}|E, M_{\mathrm{out}}) \\ &\leq \ln 2 + P_e NR, \end{aligned} \tag{2.56}$$

where we use $S(M_{\mathrm{in}}|E, M_{\mathrm{out}}) = P_e S(M_{\mathrm{in}}|E = 0, M_{\mathrm{out}}) \leq P_e S(M_{\mathrm{in}})$, and $S(E|M_{\mathrm{out}}) \leq S(E) \leq \ln 2$. This inequality (2.56) is well known as Fano's inequality.

The Markov property $p(M_{\mathrm{in}}, X, Y, M_{\mathrm{out}}) = p(M_{\mathrm{in}})p(X|M_{\mathrm{in}})p(Y|X)p(M_{\mathrm{out}}|Y)$ is satisfied in this setting. From the Markov property, we have $I(M_{\mathrm{in}} : M_{\mathrm{out}}|Y) = 0$,

$I(M_{\rm in} : Y|X) = 0$, and

$$\begin{aligned} I(M_{\rm in} : M_{\rm out}) &\le I(M_{\rm in} : Y) + I(M_{\rm in} : M_{\rm out}|Y) \\ &\le I(X : Y) + I(M_{\rm in} : Y|X) \\ &= I(X : Y) \\ &= \langle \ln p(Y) \rangle - \sum_k \langle \ln p(x_k|y_k) \rangle \\ &\le \sum_k I(x_k : y_k) \\ &\le NC. \end{aligned} \tag{2.57}$$

The inequality using the Markov property (e.g., Eq. (2.57)) is well known as the data processing inequality. From Eqs. (2.55), (2.56) and (2.57), we have

$$R \le C + \frac{\ln 2}{N} + P_e R. \tag{2.58}$$

For sufficiently large N, we have $\ln 2/N \to 0$. Thus we have proved the converse to the noisy-channel coding theorem, which indicates that the channel capacity C gives a bound of the archivable rate R with $P_e \to 0$. We add that the mutual information $I(M_{\rm in} : M_{\rm out})$ (or $I(X : Y)$) also becomes a tighter bound of the rate R with $P_e \to 0$ from Eq. (2.57).

Chapter 3

Stochastic Thermodynamics for Small System

In this chapter, let us consider a classical small system attached to a large heat bath (e.g., a Brownian particle, bio-polymer, enzyme, and molecular motor). The dynamics of the classical small system is generally described by a stochastic process (e.g., the Langevin dynamics and the Master equation). For a small system, thermodynamics in a stochastic description, so-called stochastic thermodynamics has been developed in the last two decades [70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 116, 143, 144, 145, 146, 147, 148, 149, 169, 150, 151, 152, 153, 154, 155, 156, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98]. We here introduce the stochastic thermodynamics for a small system, and the relationship between information theory and stochastic thermodynamics for a small system.

3.1 Stochastic thermodynamics

First of all, we introduce the stochastic thermodynamics, which is a framework for describing classical thermodynamic quantities such as the work, the entropy production and the heat in a stochastic level.

3.1.1 Detailed Fluctuation Theorem

Historically, the stochastic thermodynamics was numerically discovered as the fluctuation theorem by Evans *et al.* [75]. The fluctuation theorem had been proved by many researchers for a chaotic dynamics [76], a stochastic process [77], and diffusive dynamics [78]. C. Jarzynski has derived a nonequlibrium equality [80], called the Jarzynski equality or the integral fluctuation theorem, which is a generalization of the second law. G. Crooks [82] has indicated that the Jarzynski equality can be derived from the fluctuation theorem. The fluctuation theorems and the Jarzynksi equality have been confirmed experimentally for several systems such as the colloidal particle, the electric circuit and the RNA folding [89, 90, 91, 92, 93, 94, 95, 98]. Such a nonequilibrium relationship can be derived from the detailed fluctuation theorem, which is the refinement of the detailed balance property [122].

We here consider the time evolution of a system X from time t to time t'. Let $x_t = \{x_t^+, x_t^-\}$ be the phase space of a system at time t, where x_t^+ denotes an even function of the momentum (e.g., the position, and the chemical concentration) at time t, and x_t^- denotes an odd function of the momentum (e.g., the velocity, the magnetic field) at time t. If the microscopic dynamics of a system such as a Hamiltonian dynamics satisfies the reversibility, we have a detailed balance property:

$$p(x_{t'}^+, x_{t'}^- | x_t^+, x_t^-) p_{\mathrm{eq}}(x_t) = p(x_t^+, -x_t^- | x_{t'}^+, -x_{t'}^-) p_{\mathrm{eq}}(x_{t'}), \tag{3.1}$$

where p_{eq} is the equilibrium distribution. This detailed balance property Eq. (3.1) is valid for a closed, isolated and finite physical system. The detailed balance property can also be generalized to a small system interacting with multiple heat baths, and its generalization is sometimes called the detailed fluctuation theorem in the context of the fluctuation theorem [70]. For example, the Hamiltonian derivation of the detailed fluctuation theorem was given by C. Jarzynski [83].

Let T_i be the temperature of the ith heat bath, H_i be the Hamiltonian of the ith heat bath, and z_t be the phase space point of the multiple heat bathes at time t. Here we consider the time evolution of the small system x_t interacting with multiple heat baths z_t, where the interaction Hamiltonian between x_t and z_t is sufficiently small and negligible. The detailed fluctuation theorem of a small system x_t is given by

$$p(x_{t'}^+, x_{t'}^- | x_t^+, x_t^-) p_{\mathrm{eq}}(z_t) = p(x_t^+, -x_t^- | x_{t'}^+, -x_{t'}^-) p_{\mathrm{eq}}(z_{t'}), \tag{3.2}$$

$$p_{\mathrm{eq}}(z_t) = Z^{-1} \exp \left[- \sum_i \frac{H_i(z_t)}{k_B T_i} \right], \tag{3.3}$$

where k_B is the Boltzmann constant, and $Z := \int dz_t \exp[-\sum_i H_i(z_t)/(k_B T_i)]$ is the partition function. The detailed fluctuation theorem is rewritten by the entropy changes $\Delta s_{\mathrm{bath}} inthemultipleheatbaths$ such as

$$\ln \frac{p(x_{t'}|x_t)}{p_B(x_{t'}|x_t)} = \Delta s_{\mathrm{bath}}, \tag{3.4}$$

$$\Delta s_{\mathrm{bath}} := \sum_i \frac{H_i(z_t) - H_i(z_{t'})}{k_B T_i}, \tag{3.5}$$

where we introduce the backward transition probability defined as $p_B(x_{t'}|x_t) := p(x_{t'}^+, -x_{t'}^- | x_t^+, -x_t^-)$. The quantity Δs_{bath} indicates the sum of the entropy changes in multiple heat baths caused by the time evolution of the system from x_t to $x_{t'}$, because the Hamiltonian difference $H_i(z_{t'}) - H_i(z_t)$ means the heat dissipation from the system to the ith heat bath, and $[H_i(z_t) - H_i(z_{t'})]/(k_B T_i)$ gives the entropy change in the ith heat bath. The detailed fluctuation theorem states that the entropy changes in heat baths is given by the ratio between the forward transition probability p and the backward transition probability p_B.

This description of the entropy changes in the heat baths is useful even for the stochastic model where the Hamiltonian of the heat bath is not explicitly defined.

For example, we show the case of the following overdamped Langevin equation:

$$\begin{aligned}\gamma \dot{x}(t) &= -\partial_x U(x,t) + \xi^x(t),\\ \langle \xi^x(t)\rangle &= 0,\\ \langle \xi^x(t)\xi^x(t')\rangle &= 2\gamma k_B T^x \delta(t-t'),\end{aligned} \tag{3.6}$$

where γ is the friction constant, $U(x,t)$ is the time dependent inertial energy, ∂_x denotes the partial derivative symbol with respect to x, and $\xi^x(t)$ is a white Gaussian noise of the heat bath with a temperature T^x.

The stochastic differential equation (3.6) is mathematically defined as the following discretization:

$$\gamma x_{t+dt} = \gamma x_t - \partial_x U(x_t,t)dt + \sqrt{2\gamma k_B T^x}dB_t, \tag{3.7}$$

where we define $x_t := x(t)$, $x_{t+dt} := x(t+dt)$ with an infinitesimal time interval dt. $dB_t := \int_t^{t+dt} dt\xi^x(t)/\sqrt{2\gamma k_B T^x} = B_{t+dt} - B_t$ is given by a Wiener process B_t, distributed as the normal distribution:

$$p(dB_t) = \frac{1}{\sqrt{2\pi dt}} \exp\left[-\frac{(dB_t)^2}{2dt}\right]. \tag{3.8}$$

Substituting Eq. (**??**) to Eq. (3.8), we have the forward transition probability of the Langevin equation (3.6) at time t:

$$p(x_{t+dt}|x_t) = \mathcal{N}_x \exp\left[-\frac{(\gamma x_{t+dt} - \gamma x_t + \partial_x U(x_t,t)dt)^2}{4\gamma k_B T^x dt}\right] \tag{3.9}$$

$$=: \mathcal{G}(x_t; x_{t+dt}; t), \tag{3.10}$$

where $x_t := x(t)$ denotes the state at time t, and $\mathcal{N}_x$ is the normalization constant which satisfies $\int dx_{t+dt} p(x_{t+dt}|x_t) = 1$. The backward transition probability of the Langevin equation (3.6) at time $t+dt$ is defined as

$$p_B(x_t|x_{t+dt}) := \mathcal{G}(x_{t+dt}; x_t; t+dt) \tag{3.11}$$

$$= \mathcal{N}_x \exp\left[-\frac{(\gamma x_t - \gamma x_{t+dt} + \partial_x U(x_{t+dt}, t+dt)dt)^2}{4\gamma k_B T^x dt}\right]. \tag{3.12}$$

Thus, the ratio between the forward and backward transition probabilities is calculated as

$$\ln \frac{p(x_{t+dt}|x_t)}{p_B(x_t|x_{t+dt})} = \frac{1}{k_B T^x} \frac{\partial_x U(x_t,t) + \partial_x U(x_{t+dt}, t+dt)}{2}(x_{t+dt} - x_t) \tag{3.13}$$

$$= \frac{\partial_x U \circ dx(x_t,t)}{k_B T} \tag{3.14}$$

$$= \frac{(\xi^x(t) - \gamma \dot{x}(t)) \circ dx}{k_B T}, \tag{3.15}$$

where $dx = x_{t+dt} - x_t$ and $\circ$ denotes the Stratonovich integral defined as $f \circ dx(x,t) := [f(x_{t+dt}, t+dt) + f(x_t, t)](x_{t+dt} - x_t)/2$ for any function $f(x,t)$. The Stratonovich product $\partial_x U \circ dx = (\xi^x - \gamma \dot{x}) \circ dx$ gives the definition of the heat flow for the Langevin equation, which has been historically developed by K. Sekimoto [72]. Thus, the ratio $\ln[p(x_{t+dt}|x_t)/p_B(x_t|x_{t+dt})]$ can be considered as the entropy change rate in the heat bath with a temperature T^x.

3.1.2 Entropy Production

Next, we define the entropy production, which is the sum of the stochastic entropy changes in a small system and in heat baths. Let x_k be the state of the system X at time $k = 1, \ldots, N$. We assume that the dynamics of X is given by the Markov chain:

$$p(X) = p(x_1)p(x_2|x_1)\cdots p(x_N|x_{N-1}), \tag{3.16}$$

where $X := \{x_1, \ldots, x_N\}$ also denotes the stochastic trajectory of the system X. From the detailed fluctuation theorem, the entropy changes in heat baths from time k to $k+1$ is given by

$$\Delta s^k_{\text{bath}} = \ln \frac{p(x_{k+1}|x_k)}{p_B(x_k|x_{k+1})}, \tag{3.17}$$

The entropy change in a small system from time 1 to N is defined as

$$\Delta s_x := \ln p(x_1) - \ln p(x_N). \tag{3.18}$$

This ensemble average gives the Shannon entropy difference $\langle \Delta s_x \rangle = S(x_N) - S(x_1)$. The entropy production from time $k = 1$ to $k = N$ is defined as

$$\sigma := \Delta s_x + \sum_{k=1}^{N-1} \Delta s^k_{\text{bath}} \tag{3.19}$$

$$:= \ln \frac{p(x_1)p(x_2|x_1)\ldots p(x_N|x_{N-1})}{p(x_N)p_B(x_{N-1}|x_N)\cdots p_B(x_1|x_2)}. \tag{3.20}$$

Here, we consider the physical meaning of the entropy production. If the initial probability distribution $p(x_1)$ and the finial distribution $p(x_N)$ are given by the equilibrium distributions, the probability distributions are given by the inertial energy $U(x_k, k)$ and the free energy $F(k)$:

$$p(x_1) := p_{\text{eq}}(x_1) \tag{3.21}$$

$$:= \exp[\beta(F(1) - U(x_1, 1))], \tag{3.22}$$

$$p(x_N) := p_{\text{eq}}(x_N) \tag{3.23}$$

$$:= \exp[\beta(F(N) - U(x_N, N))], \tag{3.24}$$

where β denotes the inverse temperature of the heat bath. The entropy change in the bath from time $k = 1$ to $k = N$ is rewritten by the heat absorption in the small system Q such as

$$-\beta Q := \sum_{k=1}^{N-1} \Delta s_{\mathrm{bath}}^{k}. \tag{3.25}$$

Here, the inertial energy $U(x_k, k)$ and Q are stochastic variables of the path X. From the first law of thermodynamics, a stochastic work performed by the small system W is defined as

$$W := -Q - [U(x_1, 1) - U(x_N, N)]. \tag{3.26}$$

Thus, the entropy production can be rewritten by the work W and the free energy difference $\Delta F := F(N) - F(1)$, if the initial and final states are in equilibrium:

$$\sigma := \beta(W - \Delta F). \tag{3.27}$$

3.1.3 Relative Entropy and the Second Law of Thermodynamics

If the dynamics is given by the Markov chain, we generally derive the second law of thermodynamics, i.e., the ensemble average of the entropy production is nonnegative. The second law of thermodynamics is related to the nonnegativity of the relative entropy. First, we define the stochastic relative entropy $d_{\mathrm{KL}}(p(x)||q(x))$ as

$$d_{\mathrm{KL}}(p(x)||q(x)) := \ln p(x) - \ln q(x). \tag{3.28}$$

Its ensemble average gives the relative entropy and is nonnegative,

$$\langle d_{\mathrm{KL}}(p(x)||q(x)) \rangle_p = D_{\mathrm{KL}}(p(x)||q(x)) \tag{3.29}$$
$$\geq 0. \tag{3.30}$$

If the dynamics is given by the Markov chain Eq. (3.16), the entropy production is given by the stochastic relative entropy

$$\sigma = d_{\mathrm{KL}}(p(X)||p_B(X)), \tag{3.31}$$
$$p_B(X) = p(x_N) p_B(x_{N-1}|x_N) \cdots p_B(x_1|x_2), \tag{3.32}$$

where the backward path probability $p_B(X)$ satisfies the nonnegativity $p_B(X) \geq 0$ and the normalization

$$
\begin{aligned}
\sum_X p_B(X) &= \sum_{x_2,\ldots,x_N} \left[\sum_{x_1} p_B(x_1|x_2) \right] p_B(x_3|x_2) \cdots p_B(x_{N-1}|x_N) p(x_N) \\
&= \sum_{x_2,\ldots,x_N} p_B(x_3|x_2) \cdots p_B(x_{N-1}|x_N) p(x_N) \\
&= \cdots \\
&= \sum_{x_N} p(x_N) \\
&= 1.
\end{aligned} \tag{3.33}
$$

From the nonnegativity of the relative entropy Eq. (3.30), we have the nonnegativity of the ensemble average of the entropy production:

$$
\langle \sigma \rangle \geq 0, \tag{3.34}
$$

which is well known as the second law of thermodynamics [72, 74]. From the property of the relative entropy, we derive the fact that the equality holds if and only if the reversibility of the path is achieved, i.e., $p_B(X) = p(X)$. If the initial and final states are in equilibrium, we have another expression of the second law Eq. (3.34) from Eq. (3.27),

$$
\langle W \rangle \geq \Delta F, \tag{3.35}
$$

which means that the free energy difference gives a lower bound of the work.

3.1.4 Stochastic Relative Entropy and Integral Fluctuation Theorem

We here derive the nonequlibrium identity called the integral fluctuation theorem [70] or the Jarzynski equality [80] using the definition of the stochastic relative entropy. We have the following identity of the stochastic relative entropy,

$$
\begin{aligned}
\langle \exp[-d_{\mathrm{KL}}(p(x)||q(x))] \rangle_p &= \langle q(x)/p(x) \rangle_p \\
&= \sum_x q(x) \\
&= 1.
\end{aligned} \tag{3.36}
$$

In the case of a Markov chain, the entropy production is a stochastic relativity entropy, and we have the identity

$$
\langle \exp[-\sigma] \rangle = 1, \tag{3.37}
$$

which is called the integral fluctuation theorem. This integral fluctuation theorem is a generalization of the second law of thermodynamics, because the second law of thermodynamics can be derived from Eq. (3.37):

$$\exp(0) = \langle \exp(-\sigma) \rangle \tag{3.38}$$

$$\geq \exp(-\langle \sigma \rangle), \tag{3.39}$$

$$\langle \sigma \rangle \geq 0, \tag{3.40}$$

where we used Jensen's inequality Eq. (2.17) for a convex function $\exp[f(x)]$.

If we assume that initial and final states are in equilibrium, the integral fluctuation theorem can be rewritten as

$$\exp(-\beta \Delta F) = \langle \exp(-\beta W) \rangle. \tag{3.41}$$

This expression is well known as the Jarzynski equality [80]. This equality gives an exact expression of the free energy in terms of the work distribution, i.e., $\Delta F = -\beta^{-1} \ln \langle \exp(-\beta W) \rangle$.

3.2 Steady State Thermodynamics and Feedback Cooling

The integral fluctuation theorem is an identity of the stochastic relative entropy $d_{\mathrm{KL}}(p(x)||q(x))$, and the identity can be generalized by selecting the probability distribution $q(x)$ in a stochastic relative entropy $d_{\mathrm{KL}}(p(x)||q(x))$. One influential application of the identity is the generalization of the second law for a steady state, which is called the steady-state thermodynamics [86, 90, 113, 114, 115, 157, 158, 159]. Another application is a cooling process controlled by a velocity-dependent force, called the entropy pumping or feedback cooling [116, 117, 118, 119, 120, 121]. In this section, we introduce these identities in terms of the stochastic relative entropy.

3.2.1 Housekeeping Heat and Excess Heat

If a system is driven by a time-independent force, the system will reach a nonequilibrium steady state. The steady state thermodynamics is a phenomenological attempt to construct thermodynamics for a nonequilibrium steady state, which has been introduced by Oono and Paniconi [113]. For a simple Langevin model, the generalizations of the heat dissipation for a steady state (i.e., the housekeeping heat, and the excess heat) are well-defined [86]. We show that the generalizations of the heat dissipation are related to the relative entropy.

Let us consider the following one-dimensional Langevin model:

$$\begin{aligned} \gamma \dot{x}(t) &= f_{\mathrm{ex}}(x, \lambda(t)) - \partial_x U(x, \lambda(t)) + \xi^x(t), \\ \langle \xi^x(t) \rangle &= 0, \\ \langle \xi^x(t) \xi^x(t') \rangle &= 2\gamma\beta^{-1}\delta(t - t'), \end{aligned} \tag{3.42}$$

where f_{ex} is an external nonconservative force and $\lambda(t)$ is the control parameter. To generalize thermodynamics for a steady state, the nonequilibrium potential $\phi(x, \lambda)$ is defined as

$$\phi(x, \lambda) = -\ln p_{\mathrm{ss}}(x; \lambda), \tag{3.43}$$

where $p_{\rm ss}(x;\lambda)$ is the steady-state distribution for a fixed value of the control parameter λ. The mean local velocity of the nonequilibrium steady state is defined as

$$\gamma v_{\rm ss}(x,\lambda) = f_{\rm ex}(x,\lambda) - \partial_x U(x,\lambda) + \beta^{-1}\partial_x \phi(x.\lambda). \tag{3.44}$$

The housekeeping heat $Q_{\rm hk}$ is defined as

$$Q_{\rm hk} := \int dt \dot{x}(t) \circ \gamma v_{\rm ss}(x(t),\lambda(t)), \tag{3.45}$$

which is regarded as the steady heat dissipation. The conventional heat absorption Q is defined as

$$Q := -\int dt \dot{x}(t) \circ [f_{\rm ex}(x,\lambda) - \partial_x U(x,\lambda)], \tag{3.46}$$

and we can break down the dissipative heat $-Q$ into the housekeeping heat and the rest called the excess heat dissipation:

$$-Q = Q_{\rm hk} + Q_{\rm ex}, \tag{3.47}$$

$$Q_{\rm ex} := -\beta^{-1}\int dt \dot{x} \circ \partial_x \phi(x.\lambda) \tag{3.48}$$

$$= -\beta^{-1}[\Delta\phi - \int dt \dot{\lambda} \circ \partial_\lambda \phi(x.\lambda)], \tag{3.49}$$

where $\Delta\phi := \int dt\dot{\phi}$ is the nonequilibrium potential change, and we used the chain rule of the Stratonovich integral $\dot{\phi} := \dot{\lambda} \circ \partial_\lambda \phi(x.\lambda) + \dot{x} \circ \partial_x \phi(x.\lambda)$.

3.2.2 Stochastic Relative Entropy and Hatano-Sasa Identity

In this section, we show the relationship between the steady-state thermodynamics and the stochastic relative entropy. From the nonnegativity of the relative entropy, we have generalizations of the second law of thermodynamics for a steady-state. In the steady-state thermodynamics, we have two equalities and their corresponding inequalities:

$$\beta\langle Q_{\rm hk}\rangle \geq 0, \tag{3.50}$$

$$\langle \exp(-\beta Q_{\rm hk})\rangle = 1, \tag{3.51}$$

and

$$\langle \Delta\phi\rangle \geq -\beta\langle Q_{\rm ex}\rangle, \tag{3.52}$$

$$\langle \exp(-\Delta\phi - \beta Q_{\rm ex})\rangle = 1. \tag{3.53}$$

Equation (3.53) is well known as the Hatano-Sasa equality [86].

We consider the path $X = \{x_1, \ldots, x_N\}$, where $x_k := x(kdt)$ and $\lambda_k := \lambda(kdt)$ denote the state of X and the control paremeter at time $t = kdt$, respectively, with an infinitesimal time interval dt. We assume that the initial distribution is in a steady state $p_{\rm ss}(x_1)$. The path integral of the Langevin dynamics Eq. (3.42) is given by

$$p(X) = p_{\rm ss}(x_1)p(x_2|x_1)\cdots p(x_N|x_{N-1}), \tag{3.54}$$

$$p(x_{k+1}|x_k) = \mathcal{N}_x \exp\left[-\frac{(\gamma x_{k+1} - \gamma x_k - f_{\rm tot}(x_k,\lambda_k)dt)^2}{4\gamma\beta^{-1}dt}\right], \tag{3.55}$$

where $f_{\rm tot}(x,\lambda) := f_{\rm ex}(x,\lambda) - \partial_x U(x,\lambda)$ denotes the total force.

First, we derive Eqs. (3.50) and (3.51) from the stochastic relative entropy. Here, we consider an imaginary dynamics with the force $f_{\rm tot} - 2\gamma v_{\rm ss}$, which is called the dual dynamics, where the sign of the steady mean local velocity $v_{\rm ss}$ is the opposite of the sign of the original one. The dual dynamics is related to the house keeping heat and the excess heat dissipation, because the steady mean local velocity $v_{\rm ss}$ is a cause of the house keeping heat. As shown below, the house keeping heat is given by the stochastic relative entropy between probability distributions of the original dynamics and of the dual dynamics.

The forward path probability of the dual dynamics $p_D(X)$ is given by

$$p_D(X) = p_{\rm ss}(x_1)p_D(x_2|x_1)\cdots p_D(x_N|x_{N-1}), \tag{3.56}$$

$$p_D(x_{k+1}|x_k) = \mathcal{N}_x \exp\left[-\frac{(\gamma x_{k+1} - \gamma x_k - f_{\rm tot}(x_k,\lambda_k)dt + 2\gamma v_{\rm ss}(x_k,\lambda_k)dt)^2}{4\gamma\beta^{-1}dt}\right]. \tag{3.57}$$

Up to the order $o(1)$, the stochastic relative entropy $d_{\rm KL}(p(X)||p_D(X))$ is calculated as

$$d_{\rm KL}(p(X)||p_D(X)) = \beta\sum_k dt\frac{x_{k+1}-x_k}{dt}\frac{\gamma v_{\rm ss}(x_k,\lambda_k) + \gamma v_{\rm ss}(x_{k+1},\lambda_{k+1})}{2} \tag{3.58}$$

$$= \beta Q_{\rm hk}. \tag{3.59}$$

From the identity Eq. (3.36) and the nonnegativity of the relative entropy (i.e., $D_{\rm KL}(p(X)||p_D(X)) \geq 0$), we can derive the equality and inequality of the housekeeping heat Eqs. (3.50) and (3.51).

Next, we derive Eqs. (3.52) and (3.53) from the stochastic relative entropy. The backward path probability of the dual dynamics $p_{BD}(X)$ is given by

$$p_{BD}(X) = p_{\rm ss}(x_N)p_{BD}(x_{N-1}|x_N)\cdots p_{BD}(x_1|x_2), \tag{3.60}$$

$$p_{BD}(x_k|x_{k+1}) \tag{3.61}$$

$$= \mathcal{N}_x \exp\left[-\frac{(\gamma x_k - \gamma x_{k+1} - f_{\rm tot}(x_{k+1},\lambda_{k+1})dt + 2\gamma v_{\rm ss}(x_{k+1},\lambda_{k+1})dt)^2}{4\gamma\beta^{-1}dt}\right] \tag{3.62}$$

$$= \mathcal{N}_x \exp\left[-\frac{\left(\gamma x_k - \gamma x_{k+1} + f_{\rm tot}(x_{k+1},\lambda_{k+1})dt + 2\beta^{-1}\partial_x\phi(x_{k+1},\lambda_{k+1})dt\right)^2}{4\gamma\beta^{-1}dt}\right]. \tag{3.63}$$

Up to the order $o(1)$, the stochastic relative entropy $d_{\rm KL}(p(X)||p_{BD}(X))$ is calculated as

$$d_{\rm KL}(p(X)||p_{BD}(X)) = \Delta\phi - \sum_k dt \frac{x_{k+1}-x_k}{dt}\frac{\partial_x\phi(x_k,\lambda_k)+\partial_x\phi(x_{k+1},\lambda_{k+1})}{2} \tag{3.64}$$
$$= \Delta\phi + \beta Q_{\rm ex}. \tag{3.65}$$

From the identity Eq. (3.36) and the nonnegativity of the relative entropy (i.e., $D_{\rm KL}(p(X)||p_{BD}(X)) \geq 0$), we have Eqs. (3.52) and (3.53).

3.2.3 Stochastic Relative Entropy and Feedback Cooling

As a technique of the opto-mechanics, the feedback cooling (or cold damping) has been developed to reduce the fluctuation of a mechanical degree of freedom [117, 118, 119, 120, 121]. For example, to measure the spontaneous velocity of a Brownian particle, 1.5 mK cooling of a Brownian particle optically trapped in the vacuum has been achieved experimentally [120]. As a molecular refrigerator, the feedback control with the velocity-dependent force has been discussed from a thermodynamic point of view[116]. Here, we discuss the nonequilibrium identity about the feedback cooling derived by K. H. Kim and H. Qian [116] in terms of the stochastic relative entropy.

We consider the following underdamped Langevin equation:

$$\begin{aligned} m\ddot{x}(t) &= -\gamma\dot{x}(t) - \partial_x U(x(t)) + f_{\rm fb}(\dot{x}(t)) + \xi^x(t), \\ \langle \xi^x(t)\xi^x(t')\rangle &= 2\gamma k_B T^x \delta(t-t'), \\ \langle \xi^x(t)\rangle &= 0, \end{aligned} \tag{3.66}$$

where m is the mass of the particle, $f_{\rm fb}(\dot{x}(t))$ means a velocity-dependent feedback force, which generally depends on the spontaneous velocity $\dot{x}(t)$. With an infinitesimal time interval dt, we discretize the dynamical variables $x_k \equiv x(kdt)$ and $\dot{x}_k \equiv \dot{x}(kdt)$. We consider the trajectories of the position and the velocity from time $k=1$ to $k=N$, denoted as $X \equiv \{x_1,\ldots,x_N\}$ and $\dot{X} \equiv \{\dot{x}_1,\ldots,\dot{x}_N\}$, respectively. The path probability $p(X,\dot{X})$ is given by

$$p(X,\dot{X}) = p(x_1,\dot{x}_1)p(x_2,\dot{x}_2|x_1,\dot{x}_1)\cdots p(x_N,\dot{x}_N|x_{N-1},\dot{x}_{N-1}), \tag{3.67}$$

$$\begin{aligned} p(x_{k+1},\dot{x}_{k+1}|x_k,\dot{x}_k) =& \mathcal{N}\exp\left[-\frac{dt}{2m}\partial_{\dot{x}} f_{\rm tot}(\bar{x}_k,\bar{\dot{x}}_k)\right]\delta(x_{k+1}-x_k-\bar{\dot{x}}_k dt) \\ &\times \exp\left[-\frac{[m(\dot{x}_{k+1}-\dot{x}_k)+\gamma(x_{k+1}-x_k)-f_{\rm tot}(\bar{x}_k,\bar{\dot{x}}_k)dt]^2}{4\gamma k_B T^x dt}\right], \end{aligned} \tag{3.68}$$

where $\bar{x}_k := (x_{k+1}+x_k)/2$, $\bar{\dot{x}}_k := (\dot{x}_{k+1}+\dot{x}_k)dt/2$, $f_{\rm tot}(x,\dot{x}) := -\partial_x U(x) + f_{\rm fb}(\dot{x})$ and $\mathcal{N}\exp[-dt\partial_{\dot{x}} f_{\rm tot}/(2m)]$ is the normalization prefactor, i.e., the Jacobian determinant.

The backward path probability for a feedback cooling $p_B(X, \dot{X})$ is defined as

$$p_B(X, \dot{X}) = p(x_N, \dot{x}_N) p_B(x_{N-1}, \dot{x}_{N-1} | x_N, \dot{x}_N) \cdots p_B(x_1, \dot{x}_1 | x_2, \dot{x}_2), \tag{3.69}$$

$$\begin{aligned} p_B(x_k, \dot{x}_k | x_{k+1}, \dot{x}_{k+1}) =& \mathcal{N} \exp\left[\frac{dt}{2m} \partial_{\dot{x}} f_{\mathrm{tot}}(\bar{x}_k, \bar{\dot{x}}_k)\right] \delta(x_{k+1} - x_k - \bar{\dot{x}}_k dt) \\ & \times \exp\left[-\frac{[m(\dot{x}_{k+1} - \dot{x}_k) + \gamma(x_k - x_{k-1}) - f_{\mathrm{tot}}(\bar{x}_k, \bar{\dot{x}}_k) dt]^2}{4\gamma k_B T^x dt}\right], \end{aligned} \tag{3.70}$$

where the sign of the velocity in the feedback force $f_{\mathrm{tot}}(x_{k+1}, \bar{\dot{x}}_k)$ does not change in this backward process.

Up to the order $o(1)$, the stochastic relative entropy $d_{\mathrm{KL}}(p(X, \dot{X}) || p_B(X, \dot{X}))$ is calculated as

$$\begin{aligned} & d_{\mathrm{KL}}(p(X, \dot{X}) || p_B(X, \dot{X})) \\ =& \Delta s_x + \beta \sum_k dt \frac{x_{k+1} - x_k}{dt} \frac{m(\dot{x}_{k+1} - \dot{x}_k) + f_{\mathrm{tot}}(\bar{x}_k, \bar{\dot{x}}_k)}{2} \\ & - \sum_k \frac{dt}{m} \partial_{\dot{x}} f_{\mathrm{tot}}(\bar{x}_k, \bar{\dot{x}}_k) \end{aligned} \tag{3.71}$$

$$= \Delta s_x + \beta \int dt \dot{x}(t) \circ (\xi^x(t) - \gamma \dot{x}(t)) - m^{-1} \int dt \partial_{\dot{x}} f_{\mathrm{fb}}(\dot{x}(t)) \tag{3.72}$$

$$= \sigma - \Delta s_{\mathrm{pu}}, \tag{3.73}$$

where the entropy change in a bath is defined as $\Delta s_{\mathrm{bath}} := \beta \int dt \dot{x}(t) \circ (\xi^x(t) - \gamma \dot{x}(t))$, the entropy production is defined as $\sigma := \Delta s_x + \Delta s_{\mathrm{bath}}$, and the entropy pumping Δs_{pu} is defined as $\Delta s_{\mathrm{pu}} := m^{-1} \int dt \partial_{\dot{x}} f_{\mathrm{fb}}(\dot{x}(t))$. The entropy pumping Δs_{pu} can be negative the velocity-dependent force, if the velocity-dependent feedback force f_{fb} exists.

From the identity Eq. (3.36) and the nonnegativity of the relative entropy (i.e., $D_{\mathrm{KL}}(p(X, \dot{X}) || p_B(X, \dot{X})) \geq 0$), we have the identity and the generalization of the second law:

$$\langle \exp(-\sigma + \Delta s_{\mathrm{pu}}) \rangle = 1, \tag{3.74}$$

$$\langle \sigma \rangle \geq \langle \Delta s_{\mathrm{pu}} \rangle. \tag{3.75}$$

If the velocity-dependent feedback force f_{fb} exists, a lower bound of $\langle \sigma \rangle$ can be negative. Thus, the inequality (3.75) indicates that the ensemble average of the entropy production can be negative if the feedback control exists. This discussion of feedback cooling is closely related to the problem of Maxwell's demon, but this discussion of feedback cooling completely depends on the Langevin equation (3.66). In the next section, we give a general discussion of Maxwell's demon and the entropy production under a feedback control in a different and informational way.

Chapter 4

Information Thermodynamics under Feedback Control

Recently, the stochastic thermodynamics of information processing by "Maxwell's demon" has been intensively developed, leading to unified theory of thermodynamics and information [16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66]. Historically, the connection between thermodynamics and information in a small system was first discussed in the thought experiment of Maxwell's demon in the 19th century [67, 69, 110, 111, 112, 68], where Maxwell's demon is regarded as a feedback controller. With a feedback control in a small system, the second law of thermodynamics seems to be violated, i.e., the entropy production can be negative. In this chapter, we introduce the formalism of information thermodynamics for a small system under feedback control.

4.1 Feedback Control and Entropy Production

Here, we discuss thermodynamics under a feedback control with a single measurement. Let x_k be a state of a small system X and m_1 be a memory state. At time $k = 1$, a measurement of the initial state x_1 is performed and its outcome is preserved in a memory state m_1. The measurement is given by the conditional probability $p(m_1|x_1)$ and the dynamics of a small system depends on the memory state m_1 because of the effect of the feedback control. The time evolution of the system X from time $k = 1$ to $N = 1$ is given by the following path-probability:

$$p(x_2|x_1, m_1)p(x_3|x_2, m_1) \cdots p(x_N|x_{N-1}, m_1). \tag{4.1}$$

Thus, the joint probability $p(x_1, \ldots, x_N, m_1)$ is given by

$$p(x_1, \ldots, x_N, m_1) = p(x_1)p(m_1|x_1)p(x_2|x_1, m_1) \cdots p(x_N|x_{N-1}, m_1). \tag{4.2}$$

In this protocol, we consider the detailed fluctuation theorem under a feedback control. When the system X is changed from x_k to x_{k+1}, the memory state m_1 play a role of an external parameter. Thus, the detailed fluctuation theorem is modified as

$$\Delta s_{\mathrm{bath}}^k := \ln \frac{p(x_{k+1}|x_k, m_1)}{p_B(x_k|x_{k+1}, m_1)}, \tag{4.3}$$

where p_B is the probability of the backward process. The detailed fluctuation theorem is the consequence of the detailed balance property, so that the backward probability is defined as $p_B(x_k|x_{k+1}, m_1) = p(x_k^+, -x_k^-|x_{k+1}^+, -x_{k+1}^-, m_1^+, -m_1^-)$, where $x_k = \{x_k^+, x_k^-\}$ ($m_1 = \{m_1^+, m_1^-\}$), x_k^+ (m_1^+) denotes an even function of the momentum, and x_k^- (m_1^-) denotes an odd function of the momentum. The entropy production for a feedback control is defined as

$$\sigma := \ln p(x_1) - \ln p(x_N) + \sum_{k=1}^{N-1} \Delta s_{\mathrm{bath}}^k \tag{4.4}$$

$$= \ln \left[\frac{p(x_1)}{p(x_N)} \prod_{k=1}^{N-1} \frac{p(x_{k+1}|x_k, m_1)}{p_B(x_k|x_{k+1}, m_1)} \right]. \tag{4.5}$$

We stress that this entropy production is not a stochastic relative entropy, so that its ensemble average can be negative.

4.1.1 Stochastic Relative Entropy and Sagawa-Ueda Relation

We next consider the generalization of the second law for a feedback control. In the case of a feedback control, the entropy production is not a stochastic relative entropy.

Let the stochastic mutual information between X and Y be $i(X : Y) := \ln p(X, Y) - i(X)$. Its ensemble average gives the mutual information $I(X, Y) = \langle i(X : Y) \rangle$. Here, we show that the sum of the entropy production and the stochastic mutual information difference can be rewritten by the stochastic relative entropy such as

$$\sigma + i(x_1 : m_1) - i(x_N : m_1) := \ln \frac{p(x_1)p(m_1|x_1)p(x_2|x_1, m_1) \cdots p(x_N|x_{N-1}, m_1)}{p(x_N)p(m_1|x_N)p_B(x_{N-1}|x_N, m_1) \cdots p_B(x_1|x_2, m_1)}$$
$$:= d_{\mathrm{KL}}(p(x_1, \ldots, x_N, m_1)||p_B(x_1, \ldots, x_N, m_1)). \tag{4.6}$$

$$p_B(x_1, \ldots, x_N, m_1) := p(x_N)p(m_1|x_N)p_B(x_{N-1}|x_N, m_1) \cdots p_B(x_1|x_2, m_1). \tag{4.7}$$

The backward path probability p_B satisfies the normalization of the probability:

$$\sum_{x_1, ;x_N, m_1} p_B(x_1, \ldots, x_N, m_1) := \sum_{x_N, m_1} p(x_N)p(m_1|x_N)$$
$$= 1. \tag{4.8}$$

From the identity Eq. (3.36) and the nonnegativity of the relative entropy (i.e., $D_{\mathrm{KL}}(p(x_1, \ldots, x_N, m_1)||p_B(x_1, \ldots, x_N, m_1)) \geq 0$), we have the identity and the generalization of the second law:

$$\langle \exp(-\sigma + \Delta i) \rangle = 1, \tag{4.9}$$

$$\Delta i := i(x_N : m_1) - i(x_1 : m_1), \tag{4.10}$$

$$\langle \sigma \rangle \geq \Delta I, \tag{4.11}$$

$$\Delta I := I(x_N : m_1) - I(x_1 : m_1), \tag{4.12}$$

which are known as the Sagawa-Ueda relations [25, 43]. The mutual information difference ΔI gives the bound of the ensemble average of the entropy production $\langle \sigma \rangle$. In general, the mutual information difference can be negative. The equality $\langle \sigma \rangle = \Delta I$ holds if and only if the reversibility with a memory state, i.e., $p(x_1, \ldots, x_N, m_1) = p_B(x_1, \ldots, x_N, m_1)$, is achieved.

If the initial state $p(x_1)$ and the final state with a memory state $p(x_N|m_1)$ are in equilibrium:

$$p(x_1) = p_{\mathrm{eq}}(x_1), \tag{4.13}$$

$$:= \exp[\beta(F(1) - U(1, x_1))], \tag{4.14}$$

$$p(x_N|m_1) = p_{\mathrm{eq}}(x_N|m_1), \tag{4.15}$$

$$:= \exp[\beta(F(N, m_1) - U(N, x_N|m_1))], \tag{4.16}$$

the Sagawa-Ueda relation is rewritten by the free energy and the work such as

$$\langle \exp[-\beta(W(m_1) - \Delta F(m_1)) - i(x_1 : m_1)] \rangle = 1, \tag{4.17}$$

$$\beta(\langle W(m_1) \rangle - \langle \Delta F(m_1) \rangle) \geq -I(x_1 : m_1), \tag{4.18}$$

where the work $W(m)$ is defined as $W(m_1) := \beta^{-1} \sum_k \Delta s^k_{\mathrm{bath}} - (U(1, x_1) - U(N, x_N|m_1))$, and the free energy difference is given by $\Delta F(m_1) := F(N, m_1) - F(1)$. The mutual information between the initial state x_1 and the memory state m_1 gives the bound of the apparent second law violation.

4.1.2 Maxwell's Demon Interpretation of Sagawa-Ueda Relation

The Sagawa-Ueda relation describes trade off between information and thermodynamic entropy. One of the essential applications of the Sagawa-Ueda relation is the problem of Maxwell's demon, which performs a feedback control to reduce the entropy of the system.

Here, we introduce the Szilard engine, which is a minimal model of the Maxwell's demon discussed by Leo Szilard in 1929 [69], and an application of the Sagawa-Ueda relation to the Szilard engine model. The Szilard engine is given by the following five steps (see also Figure 4.1).

(i) At first, a single particle gas exists in a box with a volume V. The box is attached to the heat bath with a temperature $T = 1/(k_B \beta)$, and the probability of the position of the particle is uniformly distributed. (ii) Next, the partition is added to divide the box to two equal parts. x_1 denotes the state of the position of the particle at this step

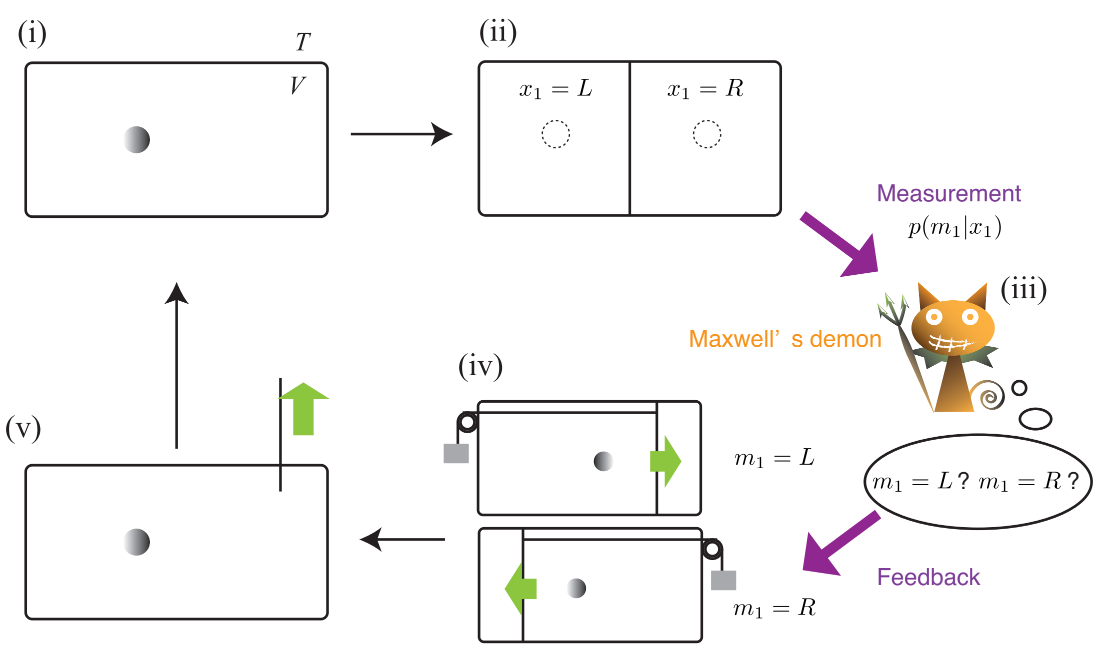

Fig. 4.1 The schematic of the Szilard's engine. Maxwell's demon measure a state of the position of a single particle x_1, and performs feedback control using the measurement outcome m_1. In a cycle, Maxwell's demon can extract the work from the heat bath attached to the box. That fact is the apparent violation of the second law of thermodynamics.

(ii), and $x_1 = L$ ($x_1 = R$) means that the particle is in the left-hand (right-hand) side of the box. The probability $p(x_1)$ is given by

$$p(x_1 = L) = \frac{1}{2}, \tag{4.19}$$

$$p(x_1 = R) = \frac{1}{2}. \tag{4.20}$$

(iii) Maxwell's demon performs a measurement of the position of the particle. In general, the measurement outcome denoted as m_1 does not coincide with the realization of the position of the particle because of the measurement error. Here, we consider that a measurement error like the binary symmetric channel such as

$$p(m_1 = L|x_1 = L) = p(m_1 = R|x_1 = R) = 1 - e, \tag{4.21}$$

$$p(m_1 = R|x_1 = L) = p(m_1 = L|x_1 = R) = e. \tag{4.22}$$

(iv) Depending on the measurement outcome m_1, Maxwell's demon quasi-statically move the partition to expand the volume of a single particle gas. The work can be extracted by this movement. (v) Finally, Maxwell's demon reduce the partition and wait for a long time to equilibrate the system,

In a cycle (i)-(v), we can extract the work at the step (iv). Nevertheless, the free energy change from (i) to (v) is zero. The entropy production in this cycle becomes negative. This apparent violation of the second law of thermodynamics has been discussed by many researchers for a long time [67], although Leo Szilard had mentioned the relationship between thermodynamic entropy and information crucially and proactively in his original paper [69]. Here, we discuss this problem of Maxwell's demon from the viewpoint of the Sagawa-Ueda relation. The Sagawa-Ueda relation gives a clear explanation of this Maxwell's demon problem in terms of the stochastic thermodynamics.

The extracted work $W_{\rm ext}(m) := -W(m)$ at the step (iv) can be calculated using the conventional thermodynamics. Let the position of the partition be $\lambda = [0,1]$, where $\lambda = 0$ denotes the left edge of the box, $\lambda = 1/2$ denotes the position at a step (ii), and $\lambda = 1$ denotes the right edge of the box. The finial position of the partition depends on the memory state m_1. The finial positions of the partition with memory states $m_1 = L$ and $m_1 = R$ denotes λ_L and λ_R, correspondingly. The final volume of the single particle gas depends on both the initial position of the particle and the final position of the partition such as

$$V_{\rm fin}(x_1 = L, m_1 = L) = V\lambda_L, \tag{4.23}$$

$$V_{\rm fin}(x_1 = R, m_1 = L) = V(1-\lambda_L), \tag{4.24}$$

$$V_{\rm fin}(x_1 = L, m_1 = R) = V\lambda_R, \tag{4.25}$$

$$V_{\rm fin}(x_1 = R, m_1 = R) = V(1-\lambda_R). \tag{4.26}$$

In a quasi-static process, the pressure of a single particle gas is maximized in any expansion of the volume, and is given by $1/(\beta V')$ with the volume of a single particle gas V'. The ensemble average of the extracted work is calculated as

$$\langle W_{\rm ext}(m_1)\rangle \leq \sum_{x_1,m_1} p(x_1,m_1) \int_{V/2}^{V_{\rm fin}(x_1,m_1)} dV' \frac{1}{\beta V'} \tag{4.27}$$

$$= \beta^{-1}\left[\frac{e}{2}\ln(2\lambda_R) + \frac{1-e}{2}\ln 2(1-\lambda_R) + \frac{e}{2}\ln(1-\lambda_L) + \frac{1-e}{2}\ln(2\lambda_L)\right] \tag{4.28}$$

$$\leq \beta^{-1}\left[\ln 2 + e\ln e + (1-e)\ln(1-e)\right]. \tag{4.29}$$

The equality holds if $\lambda_R = e$, and $\lambda_L = 1-e$ are satisfied.

The free energy difference from the step (i) to the step (v) is zero, i.e., $\langle \Delta F(m_1)\rangle = 0$. The mutual information between the initial state x_1 and the memory state is the same as the mutual information of the binary symmetric channel Eq. (2.40):

$$I(x_1 : m_1) = \ln 2 + e\ln e + (1-e)\ln(1-e). \tag{4.30}$$

Thus Eq. (4.29) becomes an example of the Sagawa-Ueda relation: $\beta(\langle W(m_1)\rangle - \langle \Delta F(m_1)\rangle \geq -I(x_1 : m_1)$.

4.2 Comparison between Sagawa-Ueda Relation and the Second Law

Here, we compare the Sagawa-Ueda relation with the second law of thermodynamics. If we consider the total system as a system X and a memory system M, the Sagawa-Ueda relation can be considered as the second law of thermodynamics for the total system X and M.

4.2.1 Total Entropy Production and Sagawa-Ueda Relation

Let us consider the Markovian dynamics of a system X and a memory system M,

$$p(X, M) = p(x_1, m_1)p(x_2, m_2|x_1, m_1) \cdots p(x_N, m_N|x_N, m_N), \tag{4.31}$$

where $(X, M) = \{(x_1, m_1), \cdots, (x_N, m_N)\}$ denotes a trajectory of the total system X and M. The entropy production of the total system σ_{XM} is defined as

$$\sigma_{XM} := \ln \frac{p(x_1, m_1)}{p(x_N, m_N)} + \sum_k \ln \frac{p(x_{k+1}, m_{k+1}|x_k, m_k)}{p_B(x_k, m_k|x_{k+1}, m_{k+1})}. \tag{4.32}$$

The entropy production σ_{XM} is a stochastic relative entropy

$$\sigma_{XM} := d_{KL}(p(X, M)||p_B(X, M)), \tag{4.33}$$

$$p_B(X, M) := p(x_N, m_N) \prod_{k=1}^{N-1} p_B(x_k, m_k|x_{k+1}, m_{k+1}), \tag{4.34}$$

so that its ensemble average is nonnegative,

$$\langle \sigma_{XM} \rangle \geq 0, \tag{4.35}$$

which is the second law of thermodynamics for the total system. We assume that the memory state M does not change in the dynamics such as

$$p(m_{k+1}|x_{k+1}, m_k, x_k) = \delta(m_k - m_{k+1}). \tag{4.36}$$

The backward process is also assumed as

$$p_B(m_k, x_k|m_{k+1}, x_{k+1}) = \delta(m_k - m_{k+1})p_B(x_k|x_{k+1}, m_{k+1}), \tag{4.37}$$

where $p_B(x_k|x_{k+1}, m_{k+1})$ denotes the backward transition probability under the condition of the memory state m_{k+1}. In case that memory state does not change, the second law of thermodynamics for the total system can be rewritten as

$$\langle \sigma_{XM} \rangle = \sum_{X,M} p(X,M) \left[\ln \frac{p(x_1,m_1)}{p(x_N,m_N)} + \sum_k \ln \frac{p(x_{k+1}|x_k,m_k)}{p_B(x_k|x_{k+1},m_{k+1})} \right] \tag{4.38}$$

$$= \sum_{X,m_1} p(x_1)p(m_1|x_1)p(x_2|x_1,m_1)p(x_2|x_1,m_2=m_1)\cdots p(x_N|x_{N-1},m_N=m_1) \tag{4.39}$$

$$\times \left[\ln \frac{p(x_1)}{p(x_N)} + \sum_k \ln \frac{p(x_{k+1}|x_k,m_k=m_1)}{p_B(x_k|x_{k+1},m_{k+1}=m_1)} + \ln \frac{p(x_1,m_1)p(x_N)}{p(x_N,m_N=m_1)p(x_1)} \right] \tag{4.40}$$

$$= \sum_{X,m_1} p(X,m_1) \left[\sigma_X + i(x_1:m_1) - i(x_N:m_1) \right] \tag{4.41}$$

$$= \langle \sigma_X \rangle + I(x_1:m_1) - I(x_N:m_1) \geq 0. \tag{4.42}$$

where $p(X,m_1) = p(x_1)p(m_1|x_1)p(x_2|x_1,m_1)\cdots p(x_N|x_{N-1},m_1)$ and the entropy production of the system X is defined as

$$\sigma_X := \ln \frac{p(x_1)}{p(x_N)} + \sum_k \ln \frac{p(x_{k+1}|x_k,m_k=m_1)}{p_B(x_k|x_{k+1},m_{k+1}=m_1)}. \tag{4.43}$$

Thus, the second law of thermodynamics for the total system Eq. (4.35) reproduces the Sagawa-Ueda relation Eq. (4.42). This fact implies that Maxwell's demon problem does not indicate the violation of the second law of thermodynamics. To consider the dynamics of the system X and the memory M, the bound of the entropy changes in heat bathes should not be the Shannon entropy change of the system $\Delta S_X := \langle \ln[p(x_1)/p(x_N)] \rangle$, but be the total Shannon entropy change $\Delta S_{XM} := \langle \ln[p(x_1,m_1)/p(x_N,m_1)] \rangle$. The difference between ΔS_{XM} and ΔS_X, gives the mutual information difference

$$I(x_1:m_1) - I(x_N:m_1) = \Delta S_{XM} - \Delta S_X. \tag{4.44}$$

Chapter 5

Bayesian Networks and Causal Networks

We next introduce the theory of a probabilistic directed acyclic graphical model well known as Bayesian networks or causal networks [102, 103, 104]. In this thesis, we construct an information thermodynamic theory on the Bayesian networks. Bayesian network itself has a long history as early as 1963 [99]. Bayesian network had been developed in 1980s [102, 100] in the context of causal modeling. By using the network, we can automatically apply Bayes' theorem to complex problems where random variables interact with each other. In recent years, Bayesian network has been intensively studied as a technique of the machine learning and pattern recognition [101]. The Bayesian network is applicable in a wide range of fields, for example, computational biology, document classification, image processing, risk analysis, financial marketing and information retrieval.

5.1 Bayesian networks

We here introduce the mathematical definition of Bayesian networks.

5.1.1 Directed Acyclic Graph

The Bayesian network is given by a directed acyclic graph. First we show the definition of a directed acyclic graph. Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be a directed graph, where $\mathcal{V}$ denotes a finite set of nodes (vertices) and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ denotes a set of edges (arcs). An element of $\mathcal{E}$ is given by an ordered pair of nodes, which have a direction associated with it. For example, we show a directed graph $\mathcal{V} = \{a_1, a_2, a_3\}$ and $\mathcal{E} = \{(a_1, a_2), (a_1, a_3)\}$ in Fig, 5.1. If $(a_j, a_{j'}) \in \mathcal{E}$, we write $a_j \to a_{j'}$ and say that $a_{j'}$ is a *child* of a_j and a_j is a *parent* of $a_{j'}$.

A directed graph is acyclic if there is no directed path $a_j \to \cdots \to a_{j'}$ with $a_j = a_{j'}$. For example, a directed graph $\mathcal{V} = \{a_1, a_2, a_3\}$ and $\mathcal{E} = \{(a_1, a_2), (a_2, a_3), (a_3, a_1)\}$ is not acyclic, because there is a directed path $a_1 \to a_2 \to a_3 \to a_1$. Because of the acyclicity, we have the ordering such that a_j cannot be a parent of $a_{j'}$ with $j > j'$. This ordering is called the *topological ordering* (or topological sorting). The topological ordering of a directed acyclic graph is not necessarily unique. For instance,

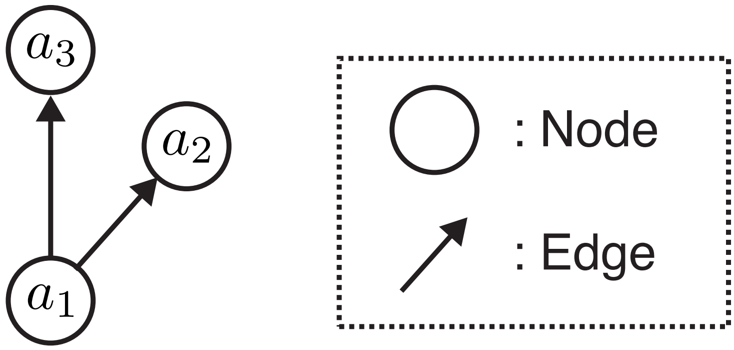

Fig. 5.1 An example of a directed graph.

in the case of a directed acyclic graph $\mathcal{V} = \{a_1, a_2, a_3\}$ and $\mathcal{E} = \{(a_1, a_2), (a_1, a_3)\}$ (Fig. 5.1), we have two topological orderings a_1, a_2, a_3 and a_1, a_3, a_2.

5.1.2 Bayesian networks

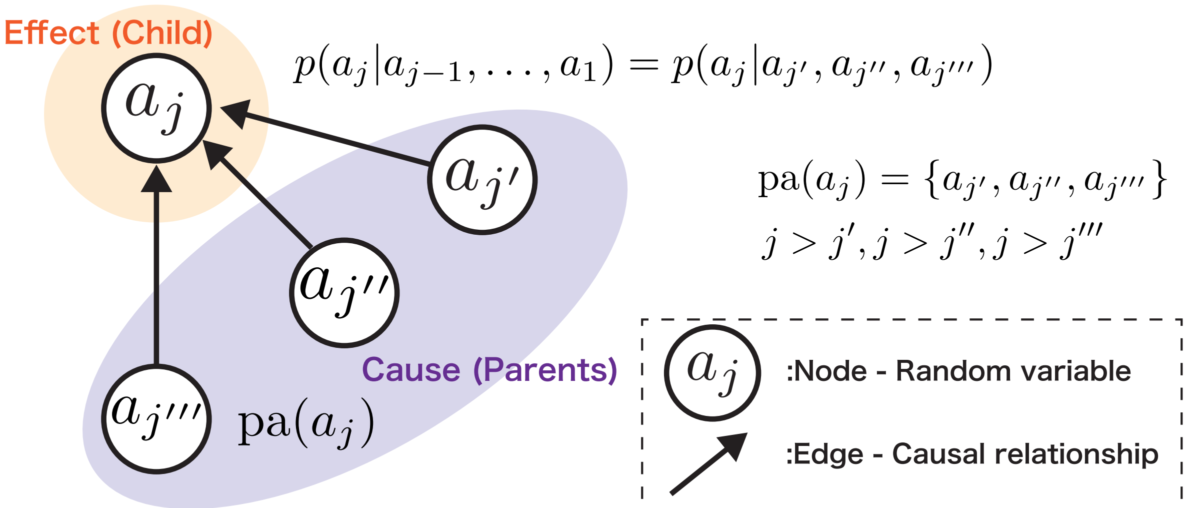

Fig. 5.2 A schematic of Bayesian network. The edge represents the causal relationship between random variables (i.e., nodes). The transition probability $p(a_j|a_{j'}, a_{j''}, a_{j'''})$ is given by the topology (edges) of the network.

We next define the Bayesian networks as a directed acyclic graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ (see also Fig. 5.2). A set of nodes $\mathcal{V} = \{a_1, \ldots, a_{N_\mathcal{V}}\}$ represents a set of random variables, where $a_1, \ldots, a_{N_\mathcal{V}}$ is a topological ordering. From the chain rule in probability theory Eq. (2.13), we have

$$p(\mathcal{V}) = p(a_1)p(a_2|a_1)p(a_3|a_2, a_1) \ldots p(a_{N_\mathcal{V}}|a_{N_\mathcal{V}-1}, \ldots, a_1). \tag{5.1}$$

On Bayesian networks, an edge $a_j \to a_{j'}$ represents a statistical dependence between a_j and $a_{j'}$. Let a set of parents of a_j be $\mathrm{pa}(a_j)$. We have $\mathrm{pa}(a_j) \subseteq \mathrm{an}(a_j)$, where

$\mathrm{an}(a_j) := \{a_1, \ldots, a_{j-1}\}$ is called *ancestors* of a_j. Statistical dependence between variables are given by the local Markov property:

$$p(a_j|\mathrm{an}(a_j)) = p(a_j|\mathrm{pa}(a_j)). \tag{5.2}$$

The local Markov property indicates that a_j and its ancestors $\mathrm{an}(a_j)$ are conditionally independent given events of its parents $\mathrm{pa}(a_j)$, because from Eq. (5.2) we have the following conditional independence,

$$p(a_j, \mathrm{an}(a_j)|\mathrm{pa}(a_j)) = p(a_j|\mathrm{pa}(a_j))p(\mathrm{an}(a_j)|\mathrm{pa}(a_j)), \tag{5.3}$$

where we used $p(a_j, \mathrm{an}(a_j)|\mathrm{pa}(a_j))/p(\mathrm{an}(a_j)|\mathrm{pa}(a_j)) = p(a_j|\mathrm{an}(a_j))$. From the local Markov property Eq. (5.2), we have a chain rule for Bayesian networks:

$$p(\mathcal{V}) = \prod_{j=1}^{N_{\mathcal{V}}} p(a_j|\mathrm{pa}(a_j)), \tag{5.4}$$

where we used $p(a_1|\mathrm{pa}(a_1)) = p(a_1|\emptyset) = p(a_1)$. [$\emptyset$ denotes an empty set.] From this chain rule Eq. (5.4), we also have $p(\mathrm{an}(a_{j+1})) = \prod_{j'=1}^{j} p(a_{j'}|\mathrm{pa}(a_{j'}))$.

We also add that $p(a_j|\mathrm{pa}(a_j), \mathcal{V}') = p(a_j|\mathrm{pa}(a_j))$ for any set $\mathcal{V}' \subseteq [\mathrm{an}(a_j) \setminus \mathrm{pa}(a_j)]$, where $\setminus$ denotes the relative complement of two sets:

$$\begin{aligned}
p(a_j|\mathrm{pa}(a_j), \mathcal{V}') &= \frac{p(a_j, \mathrm{pa}(a_j), \mathcal{V}')}{p(\mathrm{pa}(a_j), \mathcal{V}')} \\
&= \frac{\sum_{\mathrm{an}(a_{j+1})\setminus\{a_j, \mathrm{pa}(a_j), \mathcal{V}'\}} p(\mathrm{an}(a_{j+1}))}{\sum_{\mathrm{an}(a_{j+1})\setminus\{\mathrm{pa}(a_j), \mathcal{V}'\}} p(\mathrm{an}(a_{j+1}))} \\
&= \frac{[p(a_j|\mathrm{pa}(a_j))][\sum_{\mathrm{an}(a_{j+1})\setminus\{a_j, \mathrm{pa}(a_j), \mathcal{V}'\}} \prod_{j'=1}^{j-1} p(a_{j'}|\mathrm{pa}(a_{j'}))]}{[\sum_{a_j} p(a_j|\mathrm{pa}(a_j))][\sum_{\mathrm{an}(a_{j+1})\setminus\{\mathrm{pa}(a_j), \mathcal{V}'\}} \prod_{j'=1}^{j-1} p(a_{j'}|\mathrm{pa}(a_{j'}))]} \\
&= p(a_j|\mathrm{pa}(a_j)).
\end{aligned} \tag{5.5}$$

5.2 Causal Networks

Here, we introduce how the Bayesian network represents the causal relationship.

5.2.1 Causal Networks

Bayesian networks are often used to represent the causality [103]. In general, edges on Bayesian networks need not represent the causal relationship. For example, we consider a Bayesian network $\mathcal{V} = \{a_1, a_2, a_3\}$ and $\mathcal{E} = \{(a_1, a_2), (a_2, a_3)\}$ (or equivalently $a_1 \to a_2 \to a_3$). In the context of causality, we consider $a_j \to a_{j'}$ as the causal relationship from a_j to $a_{j'}$. However, a mathematical definition of this causal network is given by $p(a_1, a_2, a_3) = p(a_1)p(a_2|a_1)p(a_3|a_2)$. Using the fundamental rule, we also get

$$p(a_1, a_2, a_3) = p(a_1)p(a_2|a_1)p(a_3|a_2) \tag{5.6}$$
$$= p(a_1, a_2)\frac{p(a_3, a_2)}{p(a_2)} \tag{5.7}$$
$$= p(a_1|a_2)p(a_2)\frac{p(a_2|a_3)p(a_3)}{p(a_2)} \tag{5.8}$$
$$= p(a_3)p(a_2|a_3)p(a_1|a_2). \tag{5.9}$$

Therefore, a causal network $a_1 \to a_2 \to a_3$ reproduces exactly the same chain rule for a Bayesian network $a_3 \to a_2 \to a_1$. To discuss causal relationships using Bayesian networks, we explicitly add the causality between nodes.

J. Pearl [103] defined the *causal Bayesian networks.* In his definition of causal Bayesian networks, a probability of $\mathcal{V}$ under the condition of a constant $a_j = a$ ($a \in a_j$) is given by

$$\mathrm{Prob}_{a_j=a}(\mathcal{V}) = \prod_{j' \neq j} p(a_{j'}|\mathrm{pa}(a_{j'}))|_{a_j=a}, \tag{5.10}$$

which is known as the *truncated factorization product.* This definition indicates that the relationships should be causal.

In a physical situation, the causal network can be obtained if the topological ordering is taken as the time ordering. When the index j is in the time ordering, the transition probability of the past variable $p(a_{j'}|\mathrm{pa}(a_{j'}))$ does not depend on the realization of the future variable $a_j = a$ with $j' < j$, and Eq. (5.10) is satisfied. To discuss the causality of the physical model using Bayesian networks, we might not need to care about the precise definition of causal networks, but need to make sure that the topological ordering should be the time ordering and that the conditional probability $p(a_{j'}|\mathrm{pa}(a_{j'}))$ should be a transition probability of a physical model. Classical physical stochastic dynamics can be represented by causal networks in general, because physical dynamics holds the causality. We next introduce how to use causal networks for several physical situations.

5.2.2 Examples of Causal Networks

We show several examples of causal networks for physical situations.

5.2.2.1 Example 1: Markov chain

We consider the Markov chain $\{x_k|k = 1, \ldots, N\}$, where index k denotes the time. The the Markov chain is defined as

$$p(x_k|x_{k-1}, \ldots, x_1) = p(x_k|x_{k-1}). \tag{5.11}$$

Therefore, a causal network of the Markov chain is given by $\mathcal{V} = \{x_1, \ldots, x_N\}$ and $\mathcal{E} = \{(x_1, x_2), (x_2, x_3), \ldots, (x_{N-1}, x_N)\}$. We have $\mathrm{pa}(x_k) = x_{k-1}$ with $k \geq 2$ and $\mathrm{pa}(x_1) = \emptyset$ (see also Fig. 5.3).

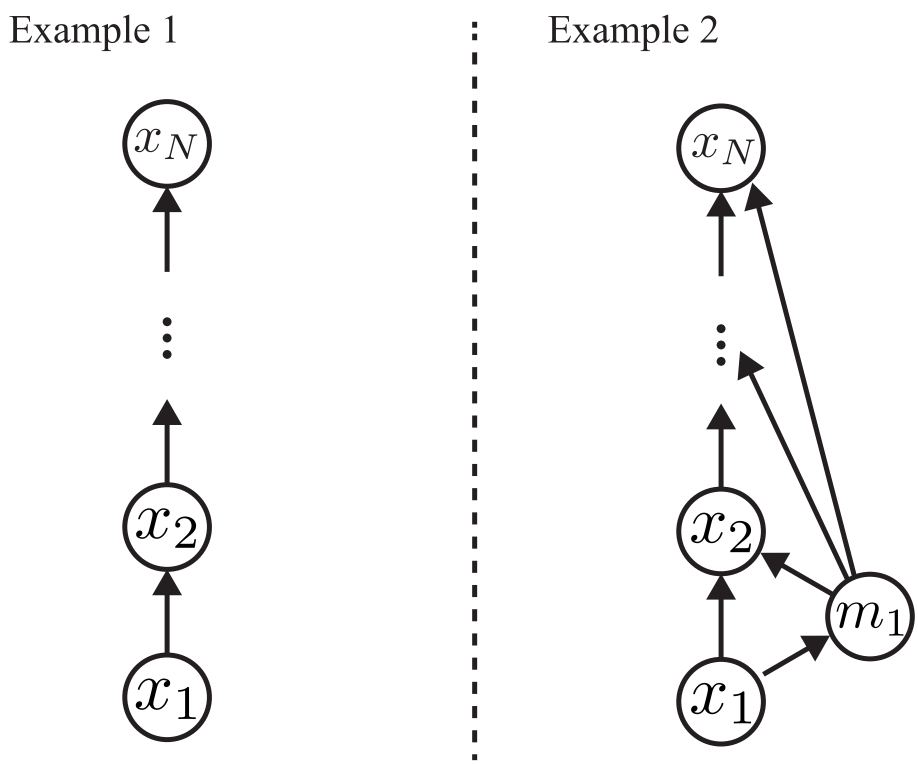

Fig. 5.3 Examples of causal networks. Example 1: Markov chain. Example 2: Feedback control with a single measurement.

5.2.2.2 Example 2: Feedback control with a single measurement

We next consider a system under feedback control with a single measurement. Let x_k be a state of a system X at time k ($k = 1, \dots, N$). At time $k = 1$, a measurement of the state x_1, which is initially distributed with a probability $p(x_1)$, is performed, and its outcome is preserved in a memory state m_1. The measurement generally includes the error and is given by the conditional probability $p(m_1|x_1)$. The outcome m_1 is used for the feedback control. The joint probability $p(x_1, \dots, x_N, m_1)$ is given by

$$p(x_1, \dots, x_N, m_1) = p(x_1)p(m_1|x_1)p(x_2|x_1, m_1)p(x_3|x_2, m_1) \cdots p(x_N|x_{N-1}, m_1). \tag{5.12}$$

Thus, a causal network of the feedback control is given by $\mathcal{V} = \{x_1, m_1, x_2, \dots, x_N\}$ and $\mathcal{E} = \{(x_1, x_2), (x_2, x_3), \dots, (x_{N-1}, x_N), (x_1, m_1), (m_1, x_2), \dots, (m_1, x_N)\}$. We have $\mathrm{pa}(x_k) = \{m_1, x_{k-1}\}$ with $k \geq 2$, $\mathrm{pa}(x_1) = \emptyset$ and $\mathrm{pa}(m_1) = x_1$ (see also Fig. 5.3).

5.2.2.3 Example 3: Repeated feedback control with multiple measurements

Here, we consider another version of feedback control. Let x_k be a state of a system X at time k ($k = 1, \dots, N$), and m_k be a memory state corresponding to x_k. At time k, a state x_k is measured by the memory state m_k with the conditional probability $p(m_k|x_k)$. The outcome m_k can be used for the feedback control after time $k+1$. The

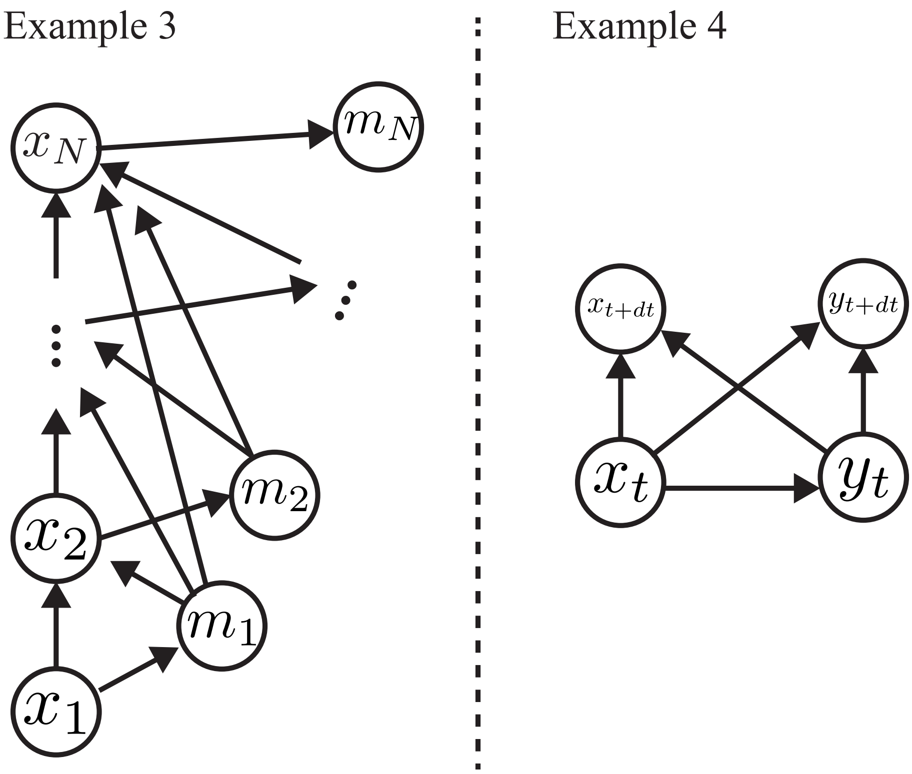

Fig. 5.4 Examples of causal networks. Example 3: Repeated feedback control with multiple measurements. Example 4: Coupled Langevin equations.

time evolution of the system X from time $k = 1$ to $N = 1$ is given by the following path-probability:

$$p(x_2|x_1, m_1)p(x_3|x_2, m_1, m_2)\cdots p(x_N|x_{N-1}, m_1, \ldots, m_{N-1}). \tag{5.13}$$

Therefore, a causal network of the repeated feedback control with multiple measurement is given by $\mathcal{V} = \{x_1, m_1, x_2, m_2, \ldots, x_N, m_N\}$ and $\mathrm{pa}(x_k) = \{m_1, \ldots, m_{k-1}, x_{k-1}\}$ with $k \geq 2$, $\mathrm{pa}(x_1) = \emptyset$ and $\mathrm{pa}(m_k) = x_k$ (see also Fig. 5.4).

5.2.2.4 Example 4: Coupled Langevin equations

The method of causal networks is applicable even for the stochastic differential equations. We consider the following coupled Langevin equations:

$$\begin{aligned}
\dot{x}(t) &= f_x(x(t), y(t)) + \xi^x(t), \\
\dot{y}(t) &= f_y(x(t), y(t)) + \xi^y(t), \\
\langle \xi^x(t) \rangle &= 0, \\
\langle \xi^y(t) \rangle &= 0, \\
\langle \xi^x(t)\xi^x(t') \rangle &= 2T^x \delta(t - t'), \\
\langle \xi^y(t)\xi^y(t') \rangle &= 2T^y \delta(t - t'), \\
\langle \xi^x(t)\xi^y(t') \rangle &= 0,
\end{aligned} \tag{5.14}$$

where $x(t)$ ($y(t)$) denotes the state of system x (y) at time t, f_x (f_y) is any force function of $x(t)$ and $y(t)$, $\xi^x(t)$ ($\xi^y(t)$) is a white Gaussian noise with zero mean and a variance $2T^x$ ($2T^y$). Noises $\xi^x(t)$ and $\xi^y(t)$ are independent such that $\langle \xi^x(t)\xi^y(t') \rangle = 0$, where $\langle \cdots \rangle$ denotes the ensemble average.

The stochastic differential equations (5.14) are mathematically defined as the following discretizations:

$$\begin{aligned}
x_{t+dt} &= x_t + f_x(x_t, y_t)dt + \sqrt{2T^x} dB_t, \\
y_{t+dt} &= y_t + f_y(x_t, y_t)dt + \sqrt{2T^y} dB'_t,
\end{aligned} \tag{5.15}$$

where we define $x_t := x(t)$, $x_{t+dt} := x(t + dt)$, $y_t := y(t)$ and $y_{t+dt} := y(t + dt)$ with an infinitesimal time interval dt. $dB_t := \int_t^{t+dt} dt \xi^x(t)/\sqrt{2T^x} = B_{t+dt} - B_t$ ($dB'_t := \int_t^{t+dt} dt \xi^y(t)/\sqrt{2T^y} = B'_{t+dt} - B'_t$) is given by a Wiener process B_t (B'_t), distributed as the normal distribution:

$$p(dB_t) = \frac{1}{\sqrt{2\pi dt}} \exp\left[-\frac{(dB_t)^2}{2dt} \right]. \tag{5.16}$$

Substituting Eq. (5.15) to Eq. (5.16), we have the Jacobian transformation of conditional probabilities:

$$p(x_{t+dt}|x_t, y_t) = \mathcal{N}_x \exp\left[-\frac{(x_{t+dt} - x_t - f_x(x_t, y_t)dt)^2}{4T^x dt} \right], \tag{5.17}$$

$$p(y_{t+dt}|x_t, y_t) = \mathcal{N}_y \exp\left[-\frac{(y_{t+dt} - y_t - f_y(x_t, y_t)dt)^2}{4T^y dt} \right], \tag{5.18}$$

where $\mathcal{N}_x := (4\pi T^x dt)^{-1/2}$ [$\mathcal{N}_y := (4\pi T^y dt)^{-1/2}$] indicates the normalization prefactor. The coupled dynamics from time t to $t + dt$ is given by the conditional probabilities Eq. (5.18). The distribution of (x_t, y_t) is generally correlated [i.e., $p(x_t, y_t) = p(x_t)p(y_t|x_t) \neq p(x_t)p(y_t)$]. Thus, the joint probability of the coupled Langevin dynamics $p(x_t, y_t, x_{t+dt}, y_{t+dt})$ is given by

$$p(x_t, y_t, x_{t+dt}, y_{t+dt}) = p(x_t)p(y_t|x_t)p(x_{t+dt}|x_t, y_t)p(y_{t+dt}|x_t, y_t). \tag{5.19}$$

A causal network which represents the Langevin dynamics Eq. (5.19) is given by $\mathcal{V} = \{x_t, y_t, x_{t+dt}, y_{t+dt}\}$, $\mathrm{pa}(x_t) = \emptyset$, $\mathrm{pa}(y_t) = x_t$, $\mathrm{pa}(x_{t+dt}) = \{x_t, y_t\}$ and $\mathrm{pa}(y_{t+dt}) = \{x_t, y_t\}$ (see also Fig. 5.4).

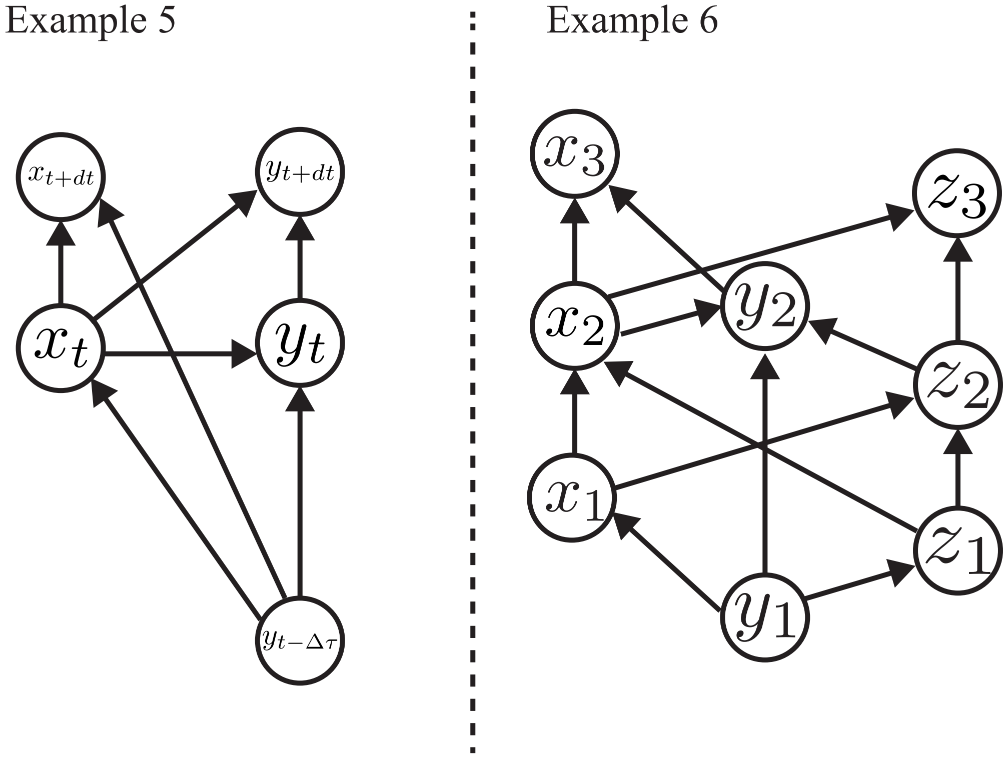

Fig. 5.5 Examples of causal networks. Example 5: Coupled dynamics with a time delay. Example 6: Complex dynamics.

5.2.2.5 Example 5: Coupled dynamics with a time delay

We note that the delayed dynamics can also be represented by a Bayesian network. Here we consider the coupled dynamics with a time delay such that

$$p(y_{t-\Delta\tau}, x_t, y_t, x_{t+dt}) = p(y_{t-\Delta\tau}, x_t, y_t) p(x_{t+dt}|x_t, y_{t-\Delta\tau}, y_t). \tag{5.20}$$

In this dynamics, the time evolution from x_t to x_{t+dt} does not depend on y_t, but depends on $y_{t-\Delta\tau}$, where $\Delta\tau$ denotes the time delay. From the chain rule in probability theory, we have

$$p(y_{t-\Delta\tau}, x_t, y_t) = p(y_{t-\Delta\tau}) p(x_t|y_{t-\Delta\tau}) p(y_t|x_t, y_{t-\Delta\tau}). \tag{5.21}$$

Thus, the time evolution of the coupled dynamics with a time delay is given by a causal network $\mathcal{V} = \{y_{t-\Delta\tau}, x_t, y_t, x_{t+dt}, y_{t+dt}\}$, $\mathrm{pa}(y_{t-\Delta\tau}) = \emptyset$, $\mathrm{pa}(x_t) = y_{t-\Delta\tau}$, $\mathrm{pa}(y_t) = \{x_t, y_{t-\Delta\tau}\}$, $\mathrm{pa}(x_{t+dt}) = \{x_t, y_{t-\Delta\tau}\}$ and $\mathrm{pa}(y_{t+dt}) = \{x_t, y_t\}$ (see also Fig. 5.5).

5.2.2.6 Example 6: Complex dynamics

We note that causal networks can generally represent the complex dynamics in multiple fluctuating systems. The causal network in Fig. 5.5 describes an example of complex three-body interactions. The causal network is given by $\mathcal{V} = \{y_1, x_1, z_1, x_2, z_2, y_2, x_3, z_3\}$, $\mathrm{pa}(y_1) = \emptyset$, $\mathrm{pa}(x_1) = y_1$, $\mathrm{pa}(z_1) = y_1$, $\mathrm{pa}(x_2) = \{x_1, z_1\}$, $\mathrm{pa}(z_2) = \{x_1, z_1\}$, $\mathrm{pa}(y_2) = \{y_1, x_2, z_2\}$, $\mathrm{pa}(x_3) = \{x_2, y_2\}$ and $\mathrm{pa}(z_3) = \{z_2, x_2\}$, where x_k (y_k, z_k) denotes the state of the system X (Y, Z) in the time ordering k. We note that time of the state x_k is not same as one of y_k. We assume that the time ordering of states is given by the topological ordering of the causal network $y_1, x_1, z_1, x_2, z_2, y_2, x_3, z_3$. The joint probability $p(\mathcal{V})$ is given by

$$\begin{aligned} p(\mathcal{V}) =& p(y_1)p(x_1|y_1)p(z_1|y_1)p(x_2|x_1, z_1) \\ & \times p(z_2|x_1, z_1)p(y_2|x_2, z_2, y_1)p(x_3|x_2, y_2)p(z_3|x_2, z_2), \end{aligned} \tag{5.22}$$

which describes the path probability of this complex dynamics in multiple fluctuating systems.

Chapter 6

Information Thermodynamics on Causal Networks

We here construct the general theory of the relationship between information and stochastic thermodynamics [50]. Characterizing complex nonequilibrium dynamics by causal networks, we derive the generalized second law of thermodynamics with information flow. This chapter is the refinement of our result [Ito S., & Sagawa T., Phys. Rev. Lett. **111**, 180503 (2013)] [50].

6.1 Entropy on Causal Networks

6.1.1 Entropy Production on Causal Networks

First of all, we clarify how to introduce the entropy production on causal networks. Let $\mathcal{V} = \{a_1, \dots, a_{N_\mathcal{V}}\}$ be a set of nodes of causal network, where a_k represents a random variable. We here introduce a set of the random variables, which represents the time evolution of the target system $X = \{x_1, \dots, x_N\}$. x_k denotes the state of the target system X at time k. X is a subset of $\mathcal{V}$, i.e., $X \subseteq \mathcal{V}$. We assume the following properties of x_k such that

$$x_{k'-1} \in \mathrm{pa}(x_k) \quad (k' = k), \tag{6.1}$$

$$x_{k'-1} \notin \mathrm{pa}(x_k) \quad (k' \neq k), \tag{6.2}$$

with $k > 2$. The former assumption indicates that the time evolution of the target system X is characterized by the sequence of edges $x_1 \to x_2 \to \cdots \to x_N$. The latter assumption corresponds to the Markov property of the physical dynamics. We stress that the latter assumption does not prohibit the non-Markovian dynamics of $\mathcal{V}$ at all. Next, we define the other system as

$$\mathcal{C} = \{c_1, \dots, c_{N'}\} := \mathcal{V} \setminus X. \tag{6.3}$$

Because c_l is an element of $\mathcal{V}$, we can rewrite c_l as $c_l = a_j$. We can introduce the time ordering of c_l from the topological ordering of $\mathcal{V}$. We assume that $l' < l$ with $j' < j$ if $c_l = a_j$ and $c_{l'} = a_{j'}$. This assumption indicates that $c_1, \dots, c_{N'}$ is ordered as the time ordering.

The probability of $p(\mathcal{V})$ is given by the chain rule of the Bayesian networks Eq. (5.4) such that

$$p(\mathcal{V}) = p(X, \mathcal{C}) \tag{6.4}$$

$$= \prod_{k=1}^{N} p(x_k|\mathrm{pa}(x_k)) \prod_{l=1}^{N'} p(c_l|\mathrm{pa}(c_l)). \tag{6.5}$$

The conditional probabilities $\prod_{k=1}^{N} p(x_k|\mathrm{pa}(x_k))$ represent the path-probability of the target system X, and the conditional probabilities $\prod_{l=1}^{N'} p(c_l|\mathrm{pa}(c_l))$ represent the path probability of the other systems $\mathcal{C}$.

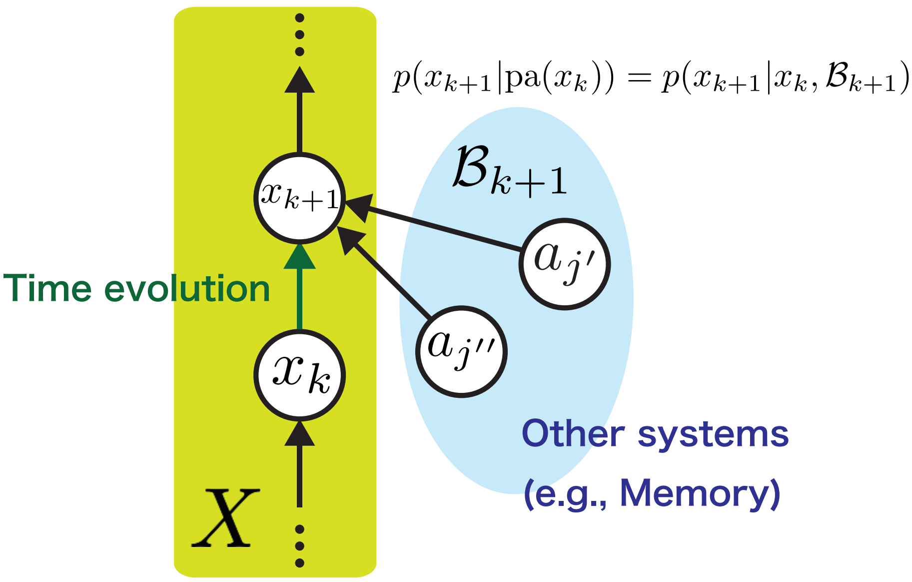

Fig. 6.1 A schematic of X and $\mathcal{B}_{k+1}$ on causal networks. $\mathcal{B}_{k+1}$ represents a set of random variables which can affects the time evolution in X from time k to $k+1$.

We introduce a set of random variables $\mathcal{B}_{k+1} := \mathrm{pa}(x_{k+1}) \setminus \{x_k\}$, which affect the time evolution of the target system X from state x_k to x_{k+1} at time k (see also Fig. 6.1). $\mathcal{B}_{k+1}$ is a subset of the variables in the other system, i.e., $\mathcal{B}_{k+1} \subseteq \mathcal{C}$. By definition of $\mathcal{B}_{k+1}$, the transition probability in X at time k is rewritten as

$$p(x_{k+1}|\mathrm{pa}(x_{k+1})) = p(x_{k+1}|x_k, \mathcal{B}_{k+1}), \tag{6.6}$$

which indicates that, in the time evolution from state x_k to x_{k+1}, $\mathcal{B}_{k+1}$ plays a role of a set of external parameters (e.g., a memory in a feedback system). Thus, the entropy change in heat baths at time k is given by

$$\Delta s^k_{\mathrm{bath}} = \ln \frac{p(x_{k+1}|x_k, \mathcal{B}_{k+1})}{p_B(x_k|x_{k+1}, \mathcal{B}_{k+1})}, \tag{6.7}$$

which is a modification of the detailed fluctuation theorem [e.g., Eq.(4.3)]. p_B describes the probability of the backward process. The definition of the backward probability is given by $p_B(x_k|x_{k+1},\mathcal{B}_{k+1}) = p(x_k^+, -x_k^-|x_{k+1}^+, -x_{k+1}^-, \mathcal{B}_{k+1}^+, -\mathcal{B}_{k+1}^-)$, where x_k^+ ($\mathcal{B}_{k+1}^+$) denotes an even function of the momentum, and x_k^- ($\mathcal{B}_{k+1}^-$) denotes an odd function of the momentum. The entropy production σ in the target system X from time $k=1$ to $k=N$ is defined as

$$\sigma := \ln p(x_1) - \ln p(x_N) + \sum_{k=1}^{N-1} \Delta s_{\mathrm{bath}}^k \tag{6.8}$$

$$= \ln\left[\frac{p(x_1)}{p(x_N)} \prod_{k=1}^{N-1} \frac{p(x_{k+1}|x_k,\mathcal{B}_{k+1})}{p_B(x_k|x_{k+1},\mathcal{B}_{k+1})}\right]. \tag{6.9}$$

6.1.2 Examples of Entropy Production on Causal Networks

We here show that the definition of the entropy production σ is well-defined in three examples (i.e., the Markov chain, the feedback control with a single measurement, and the coupled Langevin equations).

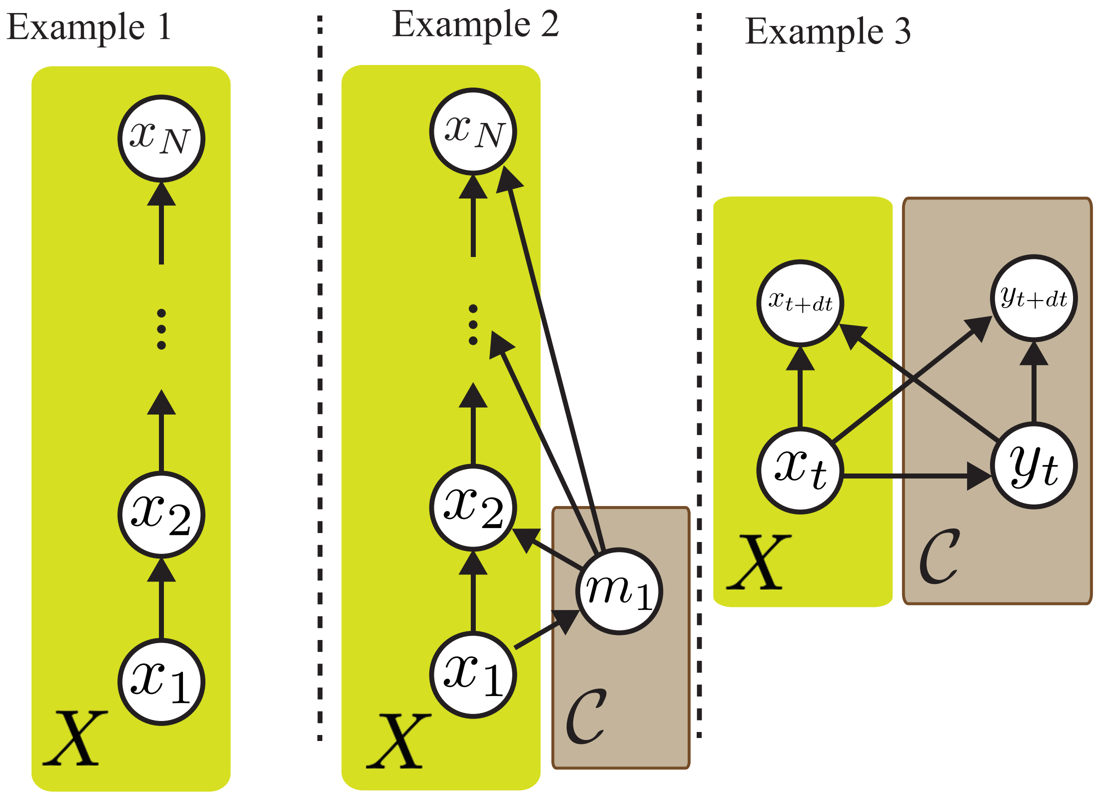

Fig. 6.2 Examples of X and $\mathcal{C}$ on causal networks. Example 1: Markov chain. Example 2: Feedback control with a single measurement. Example 3: Coupled Langevin equations.

Example 1: Markov chain
The causal network corresponding to the Markov chain is given by $\mathcal{V} = \{x_1, \ldots, x_N\}$, $\mathrm{pa}(x_k) = x_{k-1}$ with $k \geq 2$, and $\mathrm{pa}(x_1) = \emptyset$ (see also Fig. 6.2). We set $X = \{x_1, \ldots, x_N\}$ and $\mathcal{C} = \emptyset$, so that we have $\mathcal{B}_{k+1} = \mathrm{pa}(x_{k+1}) \setminus \{x_k\} = \emptyset$. Thus, the entropy production on causal networks Eq.(6.9) gives the entropy production for the Markov chain Eq. (3.20):

$$\sigma = \ln \left[\frac{p(x_1)}{p(x_N)} \prod_{k=1}^{N-1} \frac{p(x_{k+1}|x_k)}{p_B(x_k|x_{k+1})} \right]. \tag{6.10}$$

Example 2: Feedback control with a single measurement
The causal network corresponding to the system under feedback control with the single measurement is given by $\mathcal{V} = \{x_1, m_1, x_2, \ldots, x_N\}$, $\mathrm{pa}(x_k) = \{m_1, x_{k-1}\}$ with $k \geq 2$, $\mathrm{pa}(x_1) = \emptyset$, and $\mathrm{pa}(m_1) = x_1$ (see also Fig. 6.2). We set $X = \{x_1, \ldots, x_N\}$ and $\mathcal{C} = \{c_1 := m_1\}$, so that we have $\mathcal{B}_{k+1} = \mathrm{pa}(x_{k+1}) \setminus \{x_k\} = \{m_1\}$ with $k \geq 2$. Thus, the entropy production on causal networks Eq.(6.9) gives the entropy production for a feedback control Eq. (4.5):

$$\sigma = \ln \left[\frac{p(x_1)}{p(x_N)} \prod_{k=1}^{N-1} \frac{p(x_{k+1}|x_k, m_1)}{p_B(x_k|x_{k+1}, m_1)} \right]. \tag{6.11}$$

Example 3: Coupled Langevin equations
Here we discuss the following coupled Langevin equations

$$\begin{aligned}
\dot{x}(t) &= f_x(x(t), y(t)) + \xi^x(t), \\
\dot{y}(t) &= f_y(x(t), y(t)) + \xi^y(t), \\
\langle \xi^x(t) \rangle &= 0, \\
\langle \xi^y(t) \rangle &= 0, \\
\langle \xi^x(t) \xi^x(t') \rangle &= 2T^x \delta(t - t'), \\
\langle \xi^y(t) \xi^y(t') \rangle &= 2T^y \delta(t - t'), \\
\langle \xi^x(t) \xi^x(t') \rangle &= 0,
\end{aligned} \tag{6.12}$$

where x_t (y_t) is a dynamical variable of the system X (Y). The corresponding Bayesian Network is given by $\mathcal{V} = \{x_t, y_t, x_{t+dt}, y_{t+dt}\}$, $\mathrm{pa}(x_t) = \emptyset$, $\mathrm{pa}(y_t) = x_t$, $\mathrm{pa}(x_{t+dt}) = \{x_t, y_t\}$ and $\mathrm{pa}(y_{t+dt}) = \{x_t, y_t\}$ (see also Fig. 6.2). The entropy production on causal networks Eq.(6.9) gives

$$\sigma = \ln \left[\frac{p(x_t)}{p(x_{t+dt})} \frac{p(x_{t+dt}|x_t, y_t)}{p_B(x_t|x_{t+dt}, y_t)} \right], \tag{6.13}$$

where we set $X = \{x_1 := x_t, x_2 := x_{t+dt}\}$, $\mathcal{C} = \{c_1 := y_t, c_2 := y_{t+dt}\}$, and $\mathcal{B}_2 = y_t$. For the coupled Langevin dynamics, we can explicitly calculate the entropy change in heat baths $\Delta s_{\rm bath}^{k=1}$. The conditional probability $p(x_{t+dt}|x_t, y_t)$ is given by

$$p(x_{t+dt}|x_t, y_t) = \mathcal{N}_x \exp\left[-\frac{(x_{t+dt} - x_t - f_x(x_t, y_t)dt)^2}{4T^x dt}\right], \tag{6.14}$$

and the backward probability $p_B(x_{t+dt}|x_t, y_t)$ is defined as

$$p_B(x_t|x_{t+dt}, y_t) := \mathcal{N}_x \exp\left[-\frac{(x_t - x_{t+dt} - f_x(x_{t+dt}, y_t)dt)^2}{4T^x dt}\right], \tag{6.15}$$

where we assume that x_t and y_t are even functions of the momentum. Up to the order $o(dt)$, the entropy change in heat baths $\Delta s_{\rm bath}^{k=1}$ is calculated as

$$\begin{aligned}
\Delta s_{\rm bath}^{k=1} &:= \ln \frac{p(x_{t+dt}|x_t, y_t)}{p_B(x_t|x_{t+dt}, y_t)} && (6.16)\\
&= \frac{f_x(x_t, y_t) + f_x(x_{t+dt}, y_t)}{T^x}(x_{t+dt} - x_t) && (6.17)\\
&= \frac{f_x(x_t, y_t) + f_x(x_{t+dt}, y_{t+dt})}{T^x}(x_{t+dt} - x_t) && (6.18)\\
&= \frac{(\xi^x(t) - \dot{x}(t)) \circ \dot{x}(t)}{T^x}dt. && (6.19)
\end{aligned}$$

Here, $(\xi^x(t) - \dot{x}(t)) \circ \dot{x}(t)$ is Sekimoto's definition of the heat flow in the system X for the Langevin equations [72]. We add that, up to the order $o(dt)$, $\Delta s_{\rm bath}^{k=1}$ can be rewritten as

$$\begin{aligned}
\Delta s_{\rm bath}^{k=1} &= \frac{f_x(x_t, y_t) + f_x(x_{t+dt}, y_{t+dt})}{T^x}(x_{t+dt} - x_t) && (6.20)\\
&= \ln \frac{p(x_{t+dt}|x_t, y_t)}{p_B(x_t|x_{t+dt}, y_{t+dt})}, && (6.21)
\end{aligned}$$

where the backward probability is defined as

$$p_B(x_t|x_{t+dt}, y_{t+dt}) := \mathcal{N}_x \exp\left[-\frac{(x_t - x_{t+dt} - f_x(x_{t+dt}, y_{t+dt})dt)^2}{4T^x dt}\right]. \tag{6.22}$$

This fact indicates that it does not matter whether we select the condition of the backward probability y_t or y_{t+dt} if we discretize the dynamical variables with infinitesimal time interval dt.

6.1.3 Transfer Entropy on Causal Networks

We here discuss the transfer entropy on causal networks. On causal networks, we have two time series $X = \{x_1, \ldots, x_N\}$ and $\mathcal{C} = \{c_1, \ldots, c_{N'}\}$. The transfer entropy is a measure of the causal dependence in the dynamics. Thus the most natural choice of the transfer entropy from X to $\mathcal{C}$ depends on the set of parents $\mathrm{pa}(c_l)$ in the transition probability $p(c_l|\mathrm{pa}(c_l))$.

The set of parents $\mathrm{pa}(c_l)$ generally includes both elements of X and $\mathcal{C}$. We define the intersection of two sets X ($\mathcal{C}$) and $\mathrm{pa}(c_l)$ as $\mathrm{pa}_X(c_l) := X \cap \mathrm{pa}(c_l)$ ($\mathrm{pa}_{\mathcal{C}}(c_l) := \mathcal{C} \cap \mathrm{pa}(c_l)$), where $\cap$ denotes the symbol of intersection. The set of parents $\mathrm{pa}(c_l)$ is rewritten as $\mathrm{pa}(c_l) = \{\mathrm{pa}_X(c_l), \mathrm{pa}_{\mathcal{C}}(c_l)\}$, so that the transition probability $p(c_l|\mathrm{pa}(c_l))$ is calculated as

$$p(c_l|\mathrm{pa}(c_l)) = p(c_l|\mathrm{pa}_X(c_l), \mathrm{pa}_{\mathcal{C}}(c_l)) \tag{6.23}$$
$$= p(c_l|\mathrm{pa}_X(c_l), c_{l-1}, \ldots, c_1), \tag{6.24}$$

where we used the property of the Bayesian network Eq. (5.5). In the transition probability $p(c_l|\mathrm{pa}(c_l))$, the set $\mathrm{pa}_X(c_l)$ indicates the causal dependence of the target system X in the dynamics from $\{c_{l-1}, \ldots, c_1\}$ to c_l. By comparing the transition probability in $\mathcal{C}$ and that under the condition $\mathrm{pa}_X(c_l)$, we introduce the transfer entropy from X to $\mathcal{C}$ at l such as

$$I^l_{\mathrm{tr}} := \langle \ln p(c_l|\mathrm{pa}_X(c_l), c_{l-1}, \ldots, c_1) - \ln p(c_l|c_{l-1}, \ldots, c_1)\rangle \tag{6.25}$$
$$= \langle \ln p(c_l|\mathrm{pa}(c_l)) - \ln p(c_l|c_{l-1}, \ldots, c_1)\rangle. \tag{6.26}$$

This transfer entropy can be rewritten as the conditional mutual information

$$I^l_{\mathrm{tr}} = I(c_l : \mathrm{pa}_X(c_l)|c_{l-1}, \ldots, c_1). \tag{6.27}$$

From the nonnegativity of the mutual information, we have $I^l_{\mathrm{tr}} \geq 0$ with equality if and only if $p(c_l|\mathrm{pa}_X(c_l), c_{l-1}, \ldots, c_1) = p(c_l|c_{l-1}, \ldots, c_1)$ [or equivalently $\mathrm{pa}_X(c_l) = \emptyset$]. We also define the stochastic transfer entropy i^l_{tr} as

$$i^l_{\mathrm{tr}} = \ln p(c_l|\mathrm{pa}(c_l)) - \ln p(c_l|c_{l-1}, \ldots, c_1). \tag{6.28}$$

The sum of the transfer entropy $\sum_l I^l_{\mathrm{tr}}$ is a quantity similar to the directed information I^{DI}, Eq. (2.35).

6.1.4 Initial and Final Correlations on Causal Networks

We here define two types of mutual information which represent the initial and final correlations between the target system X and the outside world $\mathcal{C}$.

First, we define the initial correlation on causal networks. The initial state x_1 is initially correlated to its parents $\mathrm{pa}(x_1)$, because the state of x_1 is given by the transition probability $p(x_1|\mathrm{pa}(x_1))$. $\mathrm{pa}(x_1)$ is the set of variables in outside world, i.e., $\mathrm{pa}(x_1) \subseteq \mathcal{C}$. A natural quantification of the initial correlation between X and $\mathcal{C}$ is the mutual information between x_1 and its parents:

$$I_{\mathrm{ini}} := I(x_1 : \mathrm{pa}(x_1)). \tag{6.29}$$

From the nonnegaivitiy of the mutual information, we have $I_{\mathrm{ini}} \geq 0$ with the equality satisfied if and only if $p(x_1|\mathrm{pa}(x_1)) = p(x_1)$ [or equivalently $\mathrm{pa}(x_1) = \emptyset$].

Next, we define the final correlation on causal networks. The dynamics in the target system X generally depends on the ancestors of the final state x_N, $\mathrm{an}(x_N)$.

We introduce the set $\mathcal{C}' := \mathrm{an}(x_N) \cap \mathcal{C}$, which is the history of the outside world $\mathcal{C}$ that can affect the finial state x_N. Thus, a natural quantification of the finial correlation between X and $\mathcal{C}$ is given by the mutual information between x_N and $\mathcal{C}'$:

$$I_{\mathrm{fin}} := I(x_N : \mathcal{C}'). \tag{6.30}$$

We also define the stochastic initial correlation and the stochastic final correlation as

$$\begin{aligned} i_{\mathrm{ini}} &:= i(x_1 : \mathrm{pa}(x_1)) && (6.31)\\ &= \ln \frac{p(x_1|\mathrm{pa}(x_1))}{p(x_1)}, && (6.32)\\ i_{\mathrm{fin}} &:= i(x_N : \mathcal{C}') && (6.33)\\ &= \ln \frac{p(x_N, \mathcal{C}')}{p(x_N)p(\mathcal{C}')}, && (6.34) \end{aligned}$$

respectively.

6.2 Generalized Second Law on Causal Networks

We now state the main result of this thesis. In the foregoing setup, we have the generalized second law for subsystem X in the presence of the other system $\mathcal{C}$.

6.2.1 Relative Entropy and Generalized Second Law

Here, we define the key informational quantity Θ characterized by the topology of the causal network:

$$\Theta := i_{\mathrm{fin}} - i_{\mathrm{ini}} - \sum_{l|c_l \in \mathcal{C}'} i^l_{\mathrm{tr}}. \tag{6.35}$$

This quantity Θ indicates the total stochastic information flow from the target system X to the outside world $\mathcal{C}'$ in the dynamics from x_1 to x_N, where i_{fin} and i_{ini} mean the boundary terms. Its ensemble average $\langle\Theta\rangle$ gives the total information flow given by the mutual information and the transfer entropy.

We show that the difference between the entropy production and the informational quantity $\sigma - \Theta$ can be rewritten as the stochastic relative entropy

$$
\begin{aligned}
\sigma - \Theta =& \ln \left[\frac{p(x_1)}{p(x_N)} \prod_{k=1}^{N-1} \frac{p(x_{k+1}|x_k, \mathcal{B}_{k+1})}{p_B(x_k|x_{k+1}, \mathcal{B}_{k+1})} \right] - \ln \frac{p(x_N, \mathcal{C}')}{p(x_N)p(\mathcal{C}')} + \ln \frac{p(x_1|\mathrm{pa}(x_1))}{p(x_1)} \\
&+ \sum_{l|c_l \in \mathcal{C}'} \ln \frac{p(c_l|\mathrm{pa}(c_l))}{p(c_l|c_{l-1}, \dots, c_1)} \\
=& \ln \left[\frac{\prod_{k=1}^{N} p(x_k|\mathrm{pa}(x_k)) \prod_{l|c_l \in \mathcal{C}'} p(c_l|\mathrm{pa}(c_l))}{\prod_{k=1}^{N-1} p_B(x_k|x_{k+1}, \mathcal{B}_{k+1}) p(x_N, \mathcal{C}')} \right] \\
=& \ln \left[\frac{p(\mathcal{V})}{\prod_{k=1}^{N-1} p_B(x_k|x_{k+1}, \mathcal{B}_{k+1}) p(x_N, \mathcal{C}') \prod_{l|c_l \notin \mathcal{C}'} p(c_l|\mathrm{pa}(c_l))} \right] \\
=& d_{\mathrm{KL}}(p(\mathcal{V})||p_B(\mathcal{V})),
\end{aligned} \tag{6.36}
$$

where we define the backward path probability $p_B(\mathcal{V})$ as

$$
p_B(\mathcal{V}) = \prod_{k=1}^{N-1} p_B(x_k|x_{k+1}, \mathcal{B}_{k+1}) p(x_N, \mathcal{C}') \prod_{l|c_l \notin \mathcal{C}'} p(c_l|\mathrm{pa}(c_l)). \tag{6.37}
$$

The backward path probability satisfies the normalization of the probability such as

$$
\begin{aligned}
\sum_{\mathcal{V}} p_B(\mathcal{V}) &= \sum_{X, \mathcal{C}'} \prod_{k=1}^{N-1} p_B(x_k|x_{k+1}, \mathcal{B}_{k+1}) p(x_N, \mathcal{C}') \\
&= \sum_{x_N, \mathcal{C}'} p(x_N, \mathcal{C}') && (6.38) \\
&= 1. && (6.39)
\end{aligned}
$$

The definition of this backward path probability $p_B(\mathcal{V})$ indicates that the conditional probability in the target system X is given by the backward path probability (i.e, $\prod_{k=1}^{N-1} p_B(x_k|x_{k+1}, \mathcal{B}_{k+1})$) and the conditional probability in the other systems $\mathcal{C}$ is given by the probability distribution of the forward process (i.e, $p(x_N, \mathcal{C}') \prod_{l|c_l \notin \mathcal{C}'} p(c_l|\mathrm{pa}(c_l))$). It implies that we consider the backward path only for the target system X under the condition of stochastic variables $\mathcal{C}$, where the distribution of $\mathcal{C}$ is given by the distribution of a forward process $p(\mathcal{V})$.

From the identity Eq. (3.36) and the nonnegativity of the stochastic relative entropy $D_{\mathrm{KL}}(p(\mathcal{V})||p_B(\mathcal{V})) \geq 0$, we have the generalizations of the integral fluctuation theorem and the second law of thermodynamics,

$$
\langle \exp(-\sigma + \Theta) \rangle = 1, \tag{6.40}
$$

$$
\langle \sigma \rangle \geq I_{\mathrm{fin}} - I_{\mathrm{ini}} - \sum_{l|c_l \notin \mathcal{C}'} I_{\mathrm{tr}}^l. \tag{6.41}
$$

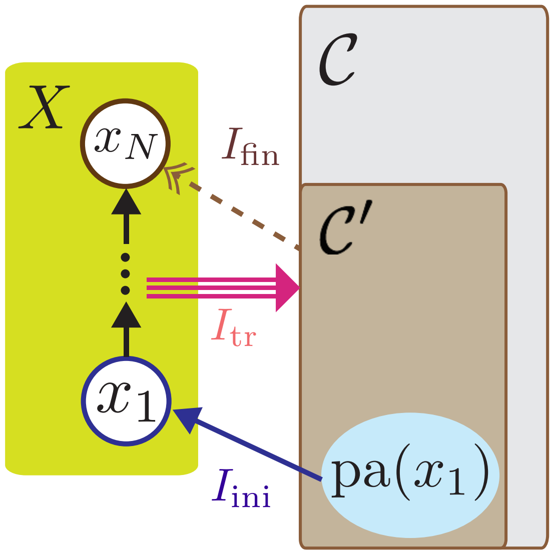

Fig. 6.3 Schematic of the generalized second law on causal networks. We consider two fluctuating subsystems X and $\mathcal{C}$. The entropy production of X is generally bounded by the informational quantity $\langle \Theta \rangle$ which includes the initial correlation $I_{\rm ini}$ between X and $\mathcal{C}$, the final correlation $I_{\rm fin}$ between them, and the transfer entropy $I_{\rm tr}$ from X to $\mathcal{C}'$ during the dynamics. We can automatically calculate the informational quantity $\langle \Theta \rangle$ using the graphical representation by causal networks.

The equality in Eq. (6.41) holds if and only if a kind of reversibility $p(\mathcal{V}) = p_B(\mathcal{V})$ holds. Application of the generalized second law to specific problems is straightforward by using the expression of the causal networks (see also Fig. 6.3). We next show several applications to stochastic models.

6.2.2 Examples of Generalized Second Law on Causal Networks

We here illustrate that the generalized integral fluctuation theorem Eq. (6.40) and the generalized second law Eq.(6.41) can reproduce known nonequilibrium relations in a unified way, and moreover can lead to novel results.

Example 1: Markov chain

We consider the causal network corresponding to the Markov chain: $\mathcal{V} := \{x_1, \ldots, x_N\}$, $\mathrm{pa}(x_k) = \{x_{k-1}\}$ with $k \geq 2$, and $\mathrm{pa}(x_1) = \emptyset$ (see also Fig. 6.4). We here set $X = \{x_1, \ldots, x_N\}$ and $\mathcal{C} = \emptyset$. We have $i_{\rm fin} = 0$, $i_{\rm ini} = 0$ and $i^l_{\rm tr} = 0$. From the generalized integral fluctuation theorem Eq. (6.40) and the generalized second law Eq.(6.41), we reproduce the conventional integral fluctuation theorem Eqs. (3.37) and (3.40):

$$\langle \exp(-\sigma) \rangle = 1, \tag{6.42}$$

$$\langle \sigma \rangle \geq 0. \tag{6.43}$$

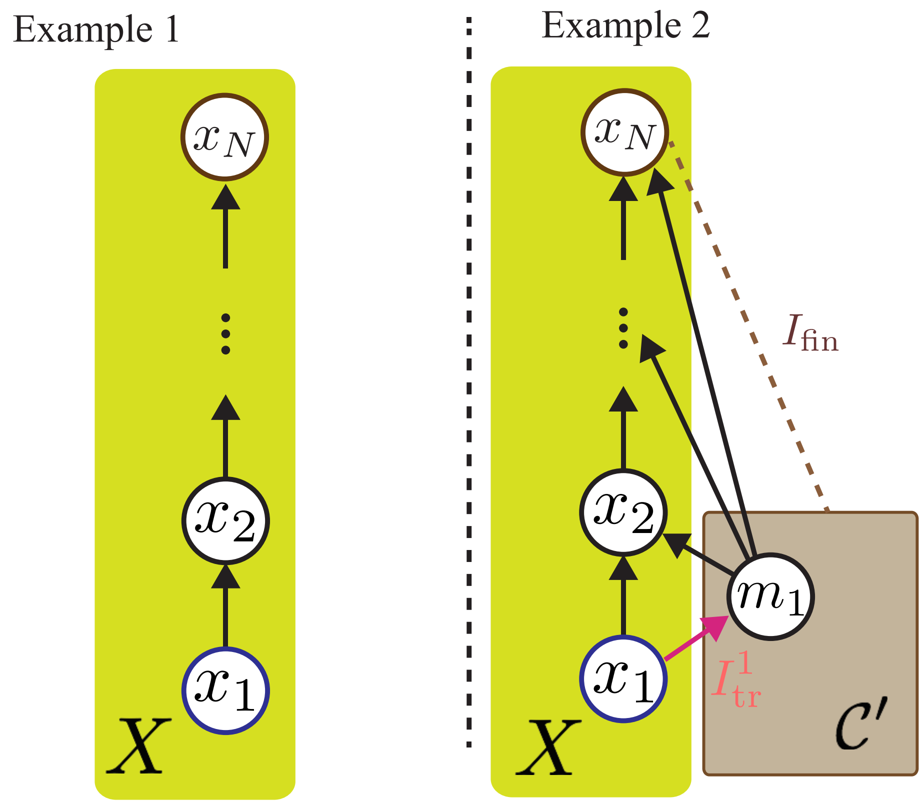

Fig. 6.4 Examples of the generalized second law on causal networks. Example 1: Markov chain. Example 2: Feedback control with a single measurement.

Example 2: Feedback control with a single measurement
We consider the causal network corresponding to the system under feedback control with a single measurement : $\mathcal{V} := \{x_1, m_1, x_2, \ldots, x_N\}$, $\mathrm{pa}(x_k) = \{x_{k-1}, m_1\}$ with $k \geq 2$, $\mathrm{pa}(m_1) = \{x_1\}$, and $\mathrm{pa}(x_1) = \emptyset$ (see also Fig. 6.4). We here set $X = \{x_1, \ldots, x_N\}$ and $\mathcal{C} = \{m_1\}$. We have $i_{\mathrm{fin}} = i(x_N : m_1)$, $i_{\mathrm{ini}} = 0$ and $i^1_{\mathrm{tr}} = i(x_1 : m_1)$. From the generalized integral fluctuation theorem Eq. (6.40) and the generalized second law Eq.(6.41), we reproduce Sagawa-Ueda relations Eqs. (4.9) and (4.11):

$$\langle \exp[-\sigma + i(x_N : m_1) - i(x_1 : m_1)] \rangle = 1, \tag{6.44}$$

$$\langle \sigma \rangle \geq I(x_N : m_1) - I(x_1 : m_1). \tag{6.45}$$

Example 3: Repeated feedback control with multiple measurement
We consider the causal network corresponding to the system under feedback control with multiple measurements : $\mathcal{V} := \{x_1, m_1, x_2, m_2, \ldots, x_N, m_N\}$, $\mathrm{pa}(x_k) = \{x_{k-1}, m_{k-1}, \ldots, m_1\}$ with $k \geq 2$, $\mathrm{pa}(m_l) = \{x_l\}$, and $\mathrm{pa}(x_1) = \emptyset$ (see also Fig. 6.5). We here set $X = \{x_1, \ldots, x_N\}$, $\mathcal{C} = \{m_1, \ldots, m_N\}$, and $\mathcal{C}' = \{m_1, \ldots, m_{N-1}\}$. We have $i_{\mathrm{fin}} = i(x_N : \{m_1, \ldots, m_{N-1}\})$, $i_{\mathrm{ini}} = 0$ and $i^l_{\mathrm{tr}} = i(x_l : m_l | m_{l-1}, \ldots, m_1)$. From the generalized integral fluctuation theorem Eq. (6.40) and the generalized

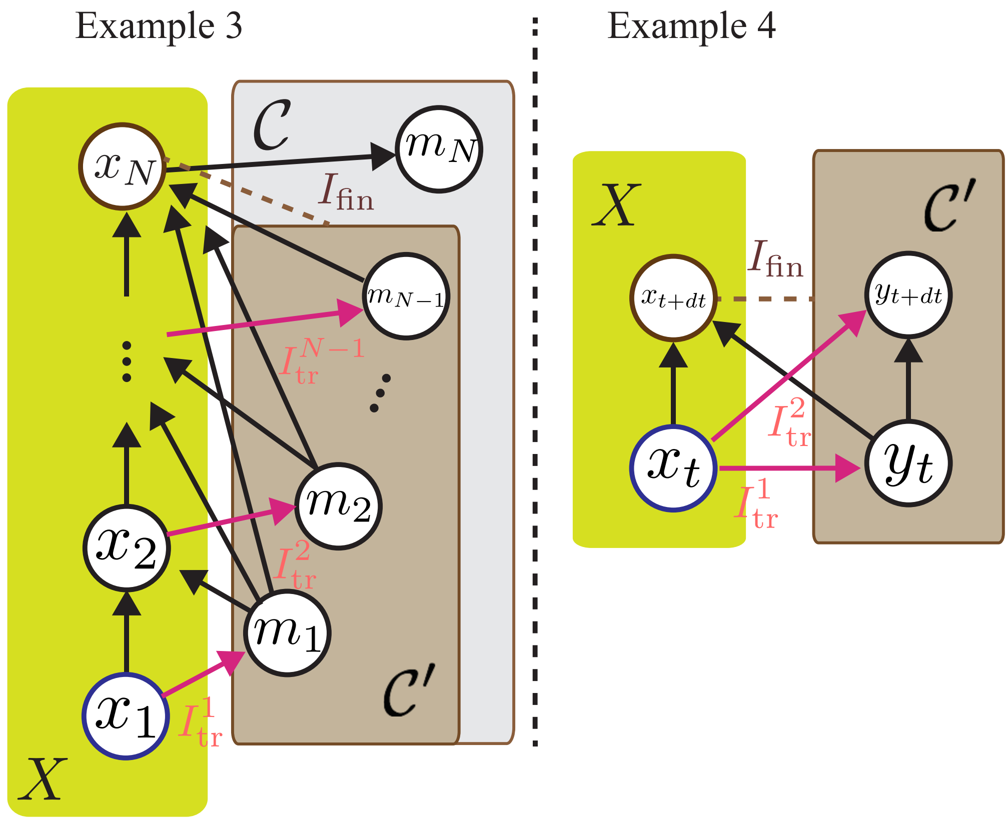

Fig. 6.5 Examples of the generalized second law on causal networks. Example 3: Repeated feedback control with multiple measurements. Example 4: Coupled Langevin equations.

second law Eq.(6.41), we have the following relations:

$$\left\langle \exp\left[-\sigma + i(x_N : \{m_1, \ldots, m_{N-1}\}) - \sum_{l=1}^{N-1} i(x_l : m_l | m_{l-1}, \ldots, m_1)\right]\right\rangle = 1, \quad (6.46)$$

$$\langle \sigma \rangle \geq I(x_N : \{m_1, \ldots, m_{N-1}\}) - \sum_{l=1}^{N-1} I(x_l : m_l | m_{l-1}, \ldots, m_1). \quad (6.47)$$

On the other hand, Horowitz and Vaikuntanathan [27] have derived the information thermodynamic equality in the case of the repeated feedback control such as

$$\left\langle \exp\left[-\beta W_d - \sum_{l=1}^{N-1} i(x_l : m_l | m_{l-1}, \ldots, m_1)\right]\right\rangle = 1, \quad (6.48)$$

where β is the inverse temperature of the heat bath, and W_d is the dissipated work defined as $\beta W_d := \sum_{k=1}^{N-1} \Delta s^k_{\text{bath}} + \ln p_{\text{eq}}(x_1) - \ln p_{\text{eq}}(x_N | m_1, \ldots, m_{N-1})$ [p_{eq} indicates the equilibrium distribution]. If the initial and final states of the system X are in thermal equilibrium, βW_d is equivalent to $\sigma - I_{\rm fin}$ such that

$$\beta W_d := \sum_{k=1}^{N-1} \Delta s^k_{\rm bath} + \ln p_{\rm eq}(x_1) - \ln p_{\rm eq}(x_N|m_1, \ldots, m_{N-1}) \tag{6.49}$$

$$= \sum_{k=1}^{N-1} \Delta s^k_{\rm bath} + \ln p_{\rm eq}(x_1) - \ln p_{\rm eq}(x_N) + i(x_N : \{m_1, \ldots, m_{N-1}\}) \tag{6.50}$$

$$= \sigma - i_{\rm fin}, \tag{6.51}$$

where we use a thermal equilibrium condition, i.e., $i(x_N : \{m_1, \ldots, m_{N-1}\}) = \ln p_{\rm eq}(x_N) - \ln p_{\rm eq}(x_N|m_1, \ldots, m_{N-1})$. Thus our general results Eqs. (6.40) and (6.41) can reproduce the known result for the system under feedback control with multiple measurements.

Example 4: Coupled Langevin equations

We consider the causal network corresponding to the coupled Langevin equations Eq. (6.12): $\mathcal{V} := \{x_t, y_t, x_{t+dt}, y_{t+dt}\}$, $\mathrm{pa}(x_{k+dt}) = \{x_t, y_t\}$, $\mathrm{pa}(y_{t+dt}) = \{x_t, y_t\}$, $\mathrm{pa}(x_t) = \emptyset$, and $\mathrm{pa}(y_t) = \{x_t\}$ (see also Fig. 6.5). We here set $X = \{x_1 := x_t, x_2 := x_{t+dt}\}$, and $\mathcal{C}' = \mathcal{C} = \{c_1 := y_t, c_2 := y_{t+dt}\}$. We have $i_{\rm fin} = i(x_{t+dt} : \{y_t, y_{t+dt}\})$, $i_{\rm ini} = 0$, $i^1_{\rm tr} = i(x_t : y_t)$, $i^2_{\rm tr} = i(x_t : y_{t+dt}|y_t)$. The informational quantity Θ is calculated as

$$\Theta = i(x_{t+dt} : \{y_t, y_{t+dt}\}) - i(x_t : y_{t+dt}|y_t) - i(x_t : y_t) \tag{6.52}$$

$$= i(x_{t+dt} : \{y_t, y_{t+dt}\}) - i(x_t : \{y_t, y_{t+dt}\}) \tag{6.53}$$

$$= i(x_{t+dt} : y_{t+dt}) - i(x_t : y_t) + i(x_{t+dt} : y_t|y_{t+dt}) - i(x_t : y_{t+dt}|y_t). \tag{6.54}$$

From the generalized integral fluctuation theorem Eq. (6.40) and the generalized second law Eq.(6.41), we have the following relations:

$$\langle \exp[-\sigma + i(x_{t+dt} : \{y_t, y_{t+dt}\}) - i(x_t : \{y_t, y_{t+dt}\})] \rangle = 1, \tag{6.55}$$

$$\langle \sigma \rangle \geq I(x_{t+dt} : \{y_t, y_{t+dt}\}) - I(x_t : \{y_t, y_{t+dt}\}), \tag{6.56}$$

or equivalently,

$$\langle \exp[-\sigma + i(x_{t+dt} : y_{t+dt}) - i(x_t : y_t) + i(x_{t+dt} : y_t|y_{t+dt}) - i(x_t : y_{t+dt}|y_t)] \rangle = 1, \tag{6.57}$$

$$\langle \sigma \rangle \geq I(x_{t+dt} : y_{t+dt}) - I(x_t : y_t) + I(x_{t+dt} : y_t|y_{t+dt}) - I(x_t : y_{t+dt}|y_t). \tag{6.58}$$

Equation (6.19) gives the entropy production σ as

$$\sigma = -\frac{j^x(t)dt}{T^x} + \ln p(x_t) - \ln p(x_{t+dt}) \tag{6.59}$$

$$j^x(t) := (\dot{x}(t) - \xi^x(t)) \circ \dot{x}(t). \tag{6.60}$$

The generalized second law Eq.(6.41) can be rewritten as

$$-\frac{\langle j^x(t) \rangle dt}{T^x} + dS_{x|y}(t) \geq I(x_{t+dt} : y_t|y_{t+dt}) - I(x_t : y_{t+dt}|y_t), \tag{6.61}$$

where $dS_{x|y}(t) := \langle \ln p(x_t|y_t) - \ln p(x_{t+dt}|y_{t+dt}) \rangle$ is the Shannon entropy difference of the system X under the condition of the system Y. The equality holds if and only if the local reversibility

$$
\begin{aligned}
&p(x_{t+dt}|x_t, y_t)p(y_{t+dt}|x_t, y_t)p(x_t, y_t) \\
=&p_B(x_t|x_{t+dt}, y_{t+dt})p(y_t|x_{t+dt}, y_{t+dt})p(x_{t+dt}, y_{t+dt})
\end{aligned}
\tag{6.62}
$$

holds.

In a stationary state, we have $p((x_{t+dt} : y_{t+dt}) = p(x_t : y_t)$, and the Shannon entropy vanishes, i.e., $dS_{x|y}(t) = 0$. Even in a stationary state, the transfer entropy from X to Y, $I(x_t : y_{t+dt}|y_t)$, and the term $I(x_{t+dt} : y_t|y_{t+dt})$ still remain. We here call $I(x_{t+dt} : y_t|y_{t+dt})$ the "backward transfer entropy", which indicates the conditional mutual information under the condition of the future variables. From the nonnegativity of the conditional mutual information, the transfer entropy $I(x_t : y_{t+dt}|y_t)$ gives an upper bound of the stationary entropy reduction in the target system X and the backward transfer entropy $I(x_{t+dt} : y_t|y_{t+dt})$ gives a lower bound of the stationary dissipation in the target system X. Thus, for the coupled dynamics, the information flow defined as the transfer entropy and backward transfer entropy from the target system to the outside world, gives a bound of the stationary heat flow $\langle j^x(t) \rangle$ in the target system.

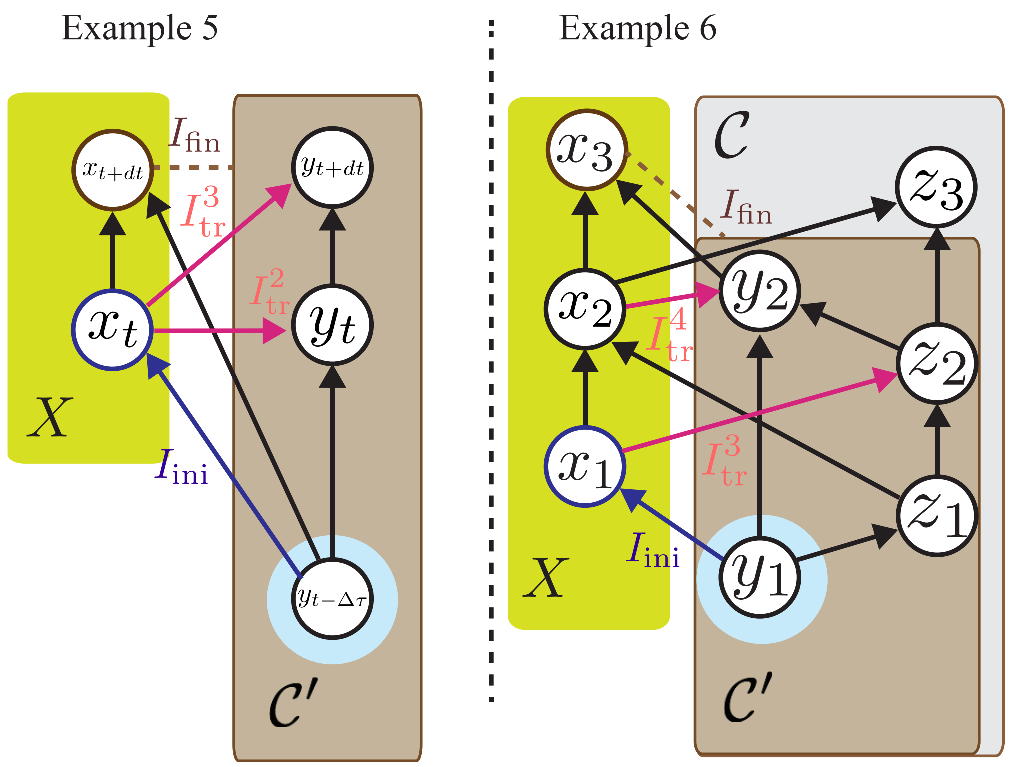

Fig. 6.6 Examples of the generalized second law on causal networks. Example 5: Coupled dynamics with a time delay. Example 6: Complex dynamics.

Example 5: Coupled dynamics with a time delay

We here consider the causal network given in Fig. 6.6: $\mathcal{V} := \{y_{t-\Delta\tau}, x_t, y_t, x_{t+dt}, y_{t+dt}\}$, $\mathrm{pa}(x_{k+dt}) = \{x_t, y_{t-\Delta\tau}\}$, $\mathrm{pa}(y_{t+dt}) = \{x_t, y_t\}$, $\mathrm{pa}(x_t) = \{y_{t-\Delta\tau}\}$, $\mathrm{pa}(y_t) = \{y_{t-\Delta\tau}, x_t\}$ and $\mathrm{pa}(y_{t-\Delta\tau}) = \emptyset$. We set $X = \{x_1 := x_t, x_2 := x_{t+dt}\}$, and $\mathcal{C} = \mathcal{C}' = \{c_1 := y_{t-\Delta\tau}, c_2 := y_t, c_3 = y_{t+dt}\}$. We have $i_{\mathrm{ini}} = i(x_t : y_{t-\Delta\tau})$, $i_{\mathrm{fin}} = i(x_{t+dt} : \{y_{t-\Delta\tau}, y_t, y_{t+dt}\})$, $i_{\mathrm{tr}}^1 = 0$, $i_{\mathrm{tr}}^2 = i(x_t : y_t | y_{t-\Delta\tau})$, and $i_{\mathrm{tr}}^2 = i(x_t : y_{t+dt} | y_t, y_{t-\Delta\tau})$. In this case, the informational quantity Θ is calculated as

$$\Theta = i(x_{t+dt} : \{y_{t-\Delta\tau}, y_t, y_{t+dt}\}) - i(x_t : y_{t-\Delta\tau}) - i(x_t : y_t | y_{t-\Delta\tau}) - i(x_t : y_{t+dt} | y_t, y_{t-\Delta\tau}) \tag{6.63}$$

$$= i(x_{t+dt} : \{y_{t-\Delta\tau}, y_t, y_{t+dt}\}) - i(x_t : \{y_{t-\Delta\tau}, y_t, y_{t+dt}\}). \tag{6.64}$$

From the generalized integral fluctuation theorem Eq. (6.40) and the generalized second law Eq.(6.41), we have the following relations:

$$\langle \exp\left[-\sigma + i(x_{t+dt} : \{y_{t-\Delta\tau}, y_t, y_{t+dt}\}) - i(x_t : \{y_{t-\Delta\tau}, y_t, y_{t+dt}\})\right] \rangle = 1, \tag{6.65}$$

$$\langle \sigma \rangle \geq I(x_{t+dt} : \{y_{t-\Delta\tau}, y_t, y_{t+dt}\}) - I(x_t : \{y_{t-\Delta\tau}, y_t, y_{t+dt}\}) \tag{6.66}$$

$$\begin{aligned} = & I(x_{t+dt} : \{y_t, y_{t+dt}\}) - I(x_t : \{y_t, y_{t+dt}\}) \\ & + I(x_{t+dt} : y_{t-\Delta\tau} | y_t, y_{t+dt}) - I(x_t : y_{t-\Delta\tau} | y_t, y_{t+dt}). \end{aligned} \tag{6.67}$$

The crucial difference between this model and the coupled Langevin equations [Example 4], is the dependence of the time delayed variable $y_{t-\Delta\tau}$. In the case of the time delayed dynamics, the mutual information difference $I(x_{t+dt} : \{y_{t-\Delta\tau}, y_t, y_{t+dt}\}) - I(x_t : \{y_{t-\Delta\tau}, y_t, y_{t+dt}\})$, which gives a bound of the entropy production, includes the variable $y_{t-\Delta\tau}$. Equation (6.67) gives the effect of the time delay for the entropy production in X as the difference of the backward transfer entropy $I(x_{t+dt} : y_{t-\Delta\tau} | y_t, y_{t+dt}) - I(x_t : y_{t-\Delta\tau} | y_t, y_{t+dt})$.

Example 6: Complex dynamics

We here consider the causal network corresponding to complex dynamics given in Fig. 6.6: $\mathcal{V} := \{y_1, x_1, z_1, x_2, z_2, y_2, x_3, z_3\}$, $\mathrm{pa}(y_1) = \emptyset$, $\mathrm{pa}(x_1) = y_1$, $\mathrm{pa}(z_1) = y_1$, $\mathrm{pa}(x_2) = \{x_1, z_1\}$, $\mathrm{pa}(z_2) = \{x_1, z_1\}$, $\mathrm{pa}(y_2) = \{y_1, x_2, z_2\}$, $\mathrm{pa}(x_3) = \{x_2, y_2\}$ and $\mathrm{pa}(z_3) = \{z_2, x_2\}$. We set $X = \{x_1, x_2, x_3\}$, $\mathcal{C} = \{c_1 := y_1, c_2 := z_1, c_3 := z_2, c_4 := y_2, c_5 := z_3\}$, and $\mathcal{C}' = \{y_1, z_1, z_2, y_2\}$. We have $i_{\mathrm{ini}} = i(x_1 : y_1)$, $i_{\mathrm{fin}} = i(x_3 : \{y_1, z_1, z_2, y_2\})$, $i_{\mathrm{tr}}^1 = 0$, $i_{\mathrm{tr}}^2 = 0$, $i_{\mathrm{tr}}^3 = i(x_1 : z_2 | y_1, z_1)$, and $i_{\mathrm{tr}}^4 = i(x_2 : y_2 | y_1, z_1, z_2)$. From the generalized integral fluctuation theorem Eq. (6.40) and the generalized second law Eq.(6.41), we have the following relations:

$$\langle \exp(-\sigma + \Theta) \rangle = 1, \tag{6.68}$$

$$\Theta = i(x_3 : \{y_1, z_1, z_2, y_2\}) - i(x_1 : y_1) - i(x_1 : z_2 | y_1, z_1) - i(x_2 : y_2 | y_1, z_1, z_2), \tag{6.69}$$

$$\langle \sigma \rangle \geq I(x_3 : \{y_1, z_1, z_2, y_2\}) - I(x_1 : y_1) - I(x_1 : z_2 | y_1, z_1) - I(x_2 : y_2 | y_1, z_1, z_2). \tag{6.70}$$

6.2.3 Coupled Chemical Reaction Model with Time-Delayed Feedback Loop

We here discuss an application of our general result to coupled chemical reaction systems with a time-delayed feedback loop. The model is characterized by a feedback loop between two systems: output system O and memory system M. We assume that each of O and M has a binary state described by 0 or 1. The model is driven by the following master equation:

$$\frac{d}{dt}p_0^X(t) = -\omega_{0,1}^X(t)p_0^X(t) + \omega_{1,0}^X(t)p_1^X(t), \tag{6.71}$$

$$\frac{d}{dt}p_1^X(t) = -\omega_{1,0}^X(t)p_1^X(t) + \omega_{0,1}^X(t)p_0^X(t). \tag{6.72}$$

where $p_0^X(t)$ (p_1^X) is the probability of the state 0 (1) with $X = O, M$ at time t. The normalization of the probability is satisfied, i.e., $p_0^X(t) + p_1^X(t) = 1$. The transition rate of a chemical reaction $\omega_{i',j'}^X$ ($i', j' = 0, 1$) is given by

$$\omega_{i',j'}^X = \frac{1}{\tau^X}\exp[-\beta^X(D_{i'j'}^X - F_{i'}^X(t))], \tag{6.73}$$

where τ^X is a time constant of the system X, β^X is the inverse temperature of a heat bath coupled to the system X, $F_{i'}^X(t)$ is the effective free energy of the state i' at time t, and $D_{i'j'}^X$ is the barrier of X between states i' and j' that satisfies $D_{i'j'}^X = D_{j'i'}^X$. This transition rate is well-established in chemical reaction models [72].

Here we consider the feedback loop between O and X (see also Fig. 6.7). We introduce the random variables (o_1, o_2, m_1, m_2), where o_1 is the state of O at time t, o_2 is the state of O at time $t+\Delta t$, m_1 is the state of M at time $t-\Delta t'$, and m_2 is the state of M at time $t+\Delta t-\Delta t'$ with $\Delta t > \Delta t'$. The feedback loop between O and X is described by the dependence of o_k and m_k in the effective free energy $F_\mu^X(t)$. From time t to $t+\Delta t$, the effective free energy $F_\mu^O(t)$ depends on m_1 and m_2, where m_1-dependence indicates the effect of a time-delayed feedback control. $F_{i'}^O(m_1, m_2)$ denotes the effective free energy of the state i' in O under the condition of (m_1, m_2). From time $t-\Delta t'$ to $t+\Delta t-\Delta t'$, the effective free energy $F_\mu^M(t)$ depends on x_1. $F_{i'}^M(x_1)$ denotes the effective free energy of the state i' in M under the condition of x_1. The joint probability distribution of this model is given by

$$p(m_1, o_1, m_2, o_2) = p(m_1, o_1)p(m_2|o_1, m_1)p(o_2|o_1, m_1, m_2). \tag{6.74}$$

The chain rule $p(m_1, o_1) = p(m_1)p(o_1|m_1)$gives the causal network corresponding to this model as $\mathcal{V} = \{m_1, o_1, m_2, o_2\}$, $\mathrm{pa}(o_2) = \{o_1, m_1, m_2\}$, $\mathrm{pa}(m_2) = \{o_1, m_1\}$, $\mathrm{pa}(o_1) = \{m_1\}$, and $\mathrm{pa}(m_1) = \emptyset$ (see also Fig. 6.8).

Information thermodynamics in the memory system M

We next treat the output system O as the target system X. If we set $M = \{x_1 := m_1, x_2 := m_2\}$, $\mathcal{C} = \{c_1 := o_1, c_2 := o_2\}$, and $\mathcal{C}' = \{o_1\}$, the entropy change $\Delta s_{\mathrm{bath}}^1$ in

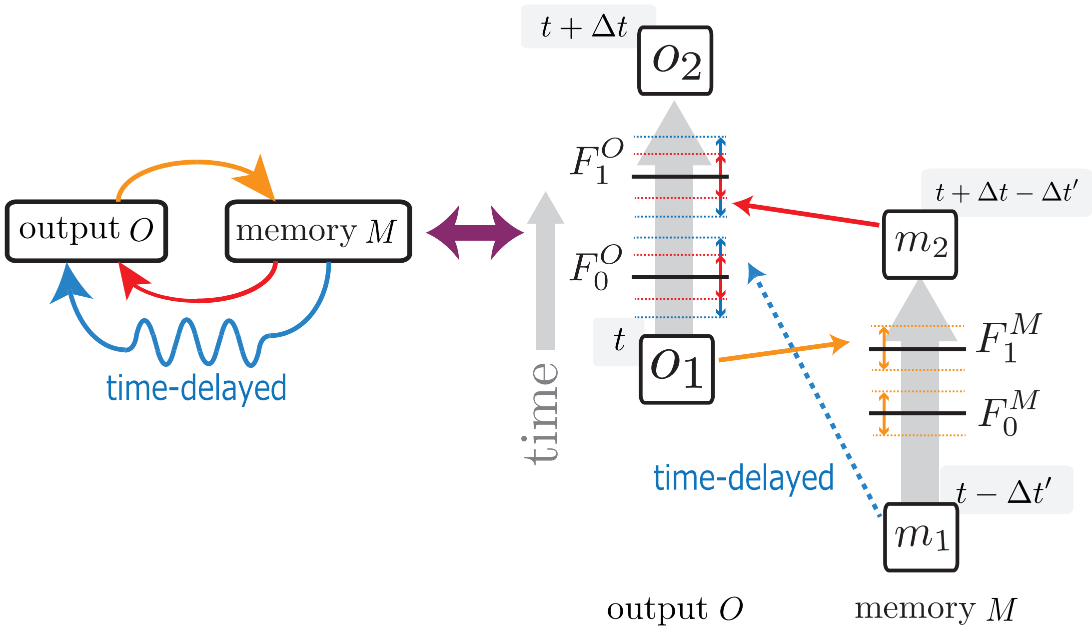

Fig. 6.7 Schematic of the coupled chemical reaction model with a time-delayed feedback loop. The previous states of O and M determine the effective free energy landscapes F^O or F^M. A blue directed arrow indicates the effect of time-delayed feedback loop. This time-delayed effect is introduced by m_1-dependence of F^O.

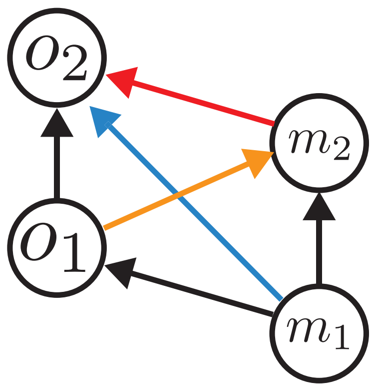

Fig. 6.8 The causal network corresponding to the coupled chemical reaction model with a time-delayed feedback loop.

a heat bath attached to the system M is given by

$$\Delta s^1_{\rm bath} = \ln \frac{p(m_2|m_1, o_1)}{p_B(m_1|m_2, o_1)}, \tag{6.75}$$

where we used $\mathcal{B}_2 = {\rm pa}(m_2)\setminus\{m_1\} = \{o_1\}$, and the backward probability is defined as $p_B(m_1 = i'|m_2 = j', o_1) := p(m_2 = i'|m_1 = j', o_1)$. From time $t-\Delta t'$ to $t+\Delta t-\Delta t'$, the master equation of the system M can be rewritten as

$$\frac{d}{dt}p_0^M(t) = -[\omega_{0,1}^M(o_1) + \omega_{1,0}^M(o_1)]p_0^O(t) + \omega_{1,0}^M(o_1), \tag{6.76}$$

$$\omega_{i',j'}^M(o_1) = \frac{1}{\tau^M}\exp[-\beta^M(D_{i'j'}^M - F_{i'}^M(o_1))], \tag{6.77}$$

and we get the solution of Eq. (6.76) as

$$p_0^M(t+\Delta t - \Delta t') = p_{0,\mathrm{eq}}^M(o_1) + (p_0^M(t-\Delta t') - p_{0,\mathrm{eq}}^M(o_1))\exp[-\omega^M(o_1)\Delta t], \tag{6.78}$$

$$p_1^M(t+\Delta t - \Delta t') = 1 - p_0^M(t+\Delta t - \Delta t'), \tag{6.79}$$

where $\omega^M(o_1) := \omega_{0,1}^M(o_1) + \omega_{1,0}^M(o_1)$, and $p_{0,\mathrm{eq}}^M(o_1)$ is an equilibrium distribution of the state 0 in M under the condition of o_1 defined as

$$p_{0,\mathrm{eq}}^M(o_1) := \frac{\exp[-\beta^M F_0^M(o_1)]}{\exp[-\beta^M F_0^M(o_1)] + \exp[-\beta^M F_1^M(o_1)]}. \tag{6.80}$$

Substituting $p_0^M(t) = 0, 1$ into the solutions of Eqs. (6.78) and (6.79), we have the conditional probability $p(m_2|m_1, o_1)$:

$$p(m_2 = 0|m_1 = 0, o_1) = p_{0,\mathrm{eq}}^M(o_1) + (1 - p_{0,\mathrm{eq}}^M(o_1))\exp[-\omega^M(o_1)\Delta t], \tag{6.81}$$

$$p(m_2 = 0|m_1 = 1, o_1) = p_{0,\mathrm{eq}}^M(o_1) - p_{0,\mathrm{eq}}^M(o_1)\exp[-\omega^M(o_1)\Delta t], \tag{6.82}$$

$$p(m_2 = 1|m_1 = i', o_1) = 1 - p(o_2 = 0|o_1 = i', o_1). \tag{6.83}$$

From Eqs. (6.81), (6.82) and (6.83), we have

$$\Delta s_{\mathrm{bath}}^2 = \ln\frac{p(m_2|m_1, o_1)}{p_B(m_1|m_2, o_1)} \tag{6.84}$$

$$= \begin{cases} 0 & (m_1 = m_2) \\ \ln[1 - p_{0,\mathrm{eq}}^M(o_1)] - \ln p_{0,\mathrm{eq}}^M(o_1) & (m_1 = 0, m_2 = 1) \\ \ln p_{0,\mathrm{eq}}^M(o_1) - \ln[1 - p_{0,\mathrm{eq}}^M(o_1)] & (m_1 = 1, m_2 = 0) \end{cases} \tag{6.85}$$

$$= -\beta^M \Delta F^M, \tag{6.86}$$

where ΔF^M is the effective free energy difference defined as $\Delta F^M := F_{m_2}^M(o_1) - F_{m_1}^O(o_1)$. The entropy change in a heat bath gives the effective free energy difference in the memory system M.

On the causal network corresponding to this model, we have $i_{\mathrm{fin}} = i(m_2 : o_1)$, $i_{\mathrm{ini}} = 0$, and $i_{\mathrm{tr}}^1 = i(m_1 : o_1)$ (see also Fig. 6.9). Informational quantity Θ is calculated as

$$\Theta = i(m_2 : o_1) - i(m_1 : o_1) \tag{6.87}$$

$$= \ln p(m_1) - \ln p(m_2) + \ln p(m_2, o_1) - \ln p(m_1, o_1). \tag{6.88}$$

From the generalized second law Eq.(6.41), we have the following relation

$$\langle\sigma\rangle \geq I(m_2 : o_1) - I(m_1 : o_1), \tag{6.89}$$

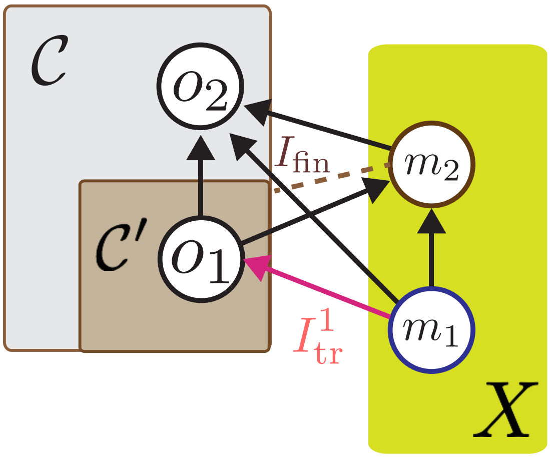

Fig. 6.9 The generalized second law in M on the causal network corresponding to the coupled chemical reaction model with a time-delayed feedback loop.

or equivalently

$$-\langle \beta^M \Delta F^M \rangle \geq \langle \ln p(m_2, o_1) \rangle - \langle \ln p(m_1, o_1) \rangle. \tag{6.90}$$

This result is equivalent to the Sagawa-Ueda relation, which is valid for a system under the feedback control. A bound of the effective free energy difference $\langle \Delta F^M \rangle$ is given by the two-body Shannon entropy difference.

Information thermodynamics in the output system O

We next treat the output system O as the target system X. If we set $X = \{x_1 := o_1, x_2 := o_2\}$ and $\mathcal{C} = \mathcal{C}' = \{c_1 := m_1, c_2 := m_2\}$, the entropy change $\Delta s^1_{\mathrm{bath}}$ in a heat bath attached to the system O is given by

$$\Delta s^1_{\mathrm{bath}} = \ln \frac{p(o_2|o_1, m_1, m_2)}{p_B(o_1|o_2, m_1, m_2)}, \tag{6.91}$$

where we used $\mathcal{B}_2 = \mathrm{pa}(x_2) \setminus \{x_1\} = \{m_1, m_2\}$, and the backward probability is defined as $p_B(o_1 = i'|o_2 = j', m_1, m_2) := p(o_2 = i'|o_1 = j', m_1, m_2)$. To obtain the analytical expression of $\Delta s^1_{\mathrm{bath}}$, we here calculate the conditional probability $p(o_2|o_1, m_1, m_2)$. From time t to $t + \Delta t$, the master equation of the system O can be rewritten as

$$\frac{d}{dt} p^O_0(t) = -[\omega^O_{0,1}(m_1, m_2) + \omega^O_{1,0}(m_1, m_2)] p^O_0(t) + \omega^O_{1,0}(m_1, m_2), \tag{6.92}$$

$$\omega^O_{i',j'}(m_1, m_2) = \frac{1}{\tau^O} \exp[-\beta^O (D^O_{i'j'} - F^O_{i'}(m_1, m_2))], \tag{6.93}$$

and we get the solution of Eq. (6.92) as

$$p^O_0(t + \Delta t) = p^O_{0,\mathrm{eq}}(m_1, m_2) + (p^O_0(t) - p^O_{0,\mathrm{eq}}(m_1, m_2)) \exp[-\omega^O(m_1, m_2)\Delta t], \tag{6.94}$$

$$p^O_1(t + \Delta t) = 1 - p^O_0(t + \Delta t), \tag{6.95}$$

where $\omega^O(m_1, m_2) := \omega^O_{0,1}(m_1, m_2) + \omega^O_{1,0}(m_1, m_2)$, and $p^O_{0,\mathrm{eq}}(m_1, m_2)$ is an equilibrium distribution of the state 0 in O under the condition of (m_1, m_2) defined as

$$p^O_{0,\mathrm{eq}}(m_1, m_2) := \frac{\exp[-\beta^O F^O_0(m_1, m_2)]}{\exp[-\beta^O F^O_0(m_1, m_2)] + \exp[-\beta^O F^O_1(m_1, m_2)]}. \tag{6.96}$$

Substituting $p^O_0(t) = 0, 1$ into the solutions of Eqs. (6.94) and (6.95), we have the conditional probability $p(o_2|o_1, m_1, m_2)$:

$$p(o_2 = 0|o_1 = 0, m_1, m_2) = p^O_{0,\mathrm{eq}}(m_1, m_2) + \left(1 - p^O_{0,\mathrm{eq}}(m_1, m_2)\right) \exp\left[-\omega^O(m_1, m_2)\Delta t\right] \tag{6.97}$$

$$p(o_2 = 0|o_1 = 1, m_1, m_2) = p^O_{0,\mathrm{eq}}(m_1, m_2) - p^O_{0,\mathrm{eq}}(m_1, m_2) \exp\left[-\omega^O(m_1, m_2)\Delta t\right] \tag{6.98}$$

$$p(o_2 = 1|o_1 = i', m_1, m_2) = 1 - p(o_2 = 0|o_1 = i', m_1, m_2). \tag{6.99}$$

From Eqs. (6.97), (6.98) and (6.99), we have

$$\Delta s^2_{\mathrm{bath}} = \ln \frac{p(o_2|o_1, m_1, m_2)}{p_B(o_1|o_2, m_1, m_2)} \tag{6.100}$$

$$= \begin{cases} 0 & (o_1 = o_2) \\ \ln[1 - p^O_{0,\mathrm{eq}}(m_1, m_2)] - \ln p^O_{0,\mathrm{eq}}(m_1, m_2) & (o_1 = 0, o_2 = 1) \\ \ln p^O_{0,\mathrm{eq}}(m_1, m_2) - \ln[1 - p^O_{0,\mathrm{eq}}(m_1, m_2)] & (o_1 = 1, o_2 = 0) \end{cases} \tag{6.101}$$

$$= -\beta^O \Delta F^O, \tag{6.102}$$

where ΔF^O is the effective free energy difference defined as $\Delta F^O := F^O_{o_2}(m_1, m_2) - F^O_{o_1}(m_1, m_2)$. The entropy change in a heat bath gives the effective free energy difference in the output system O.

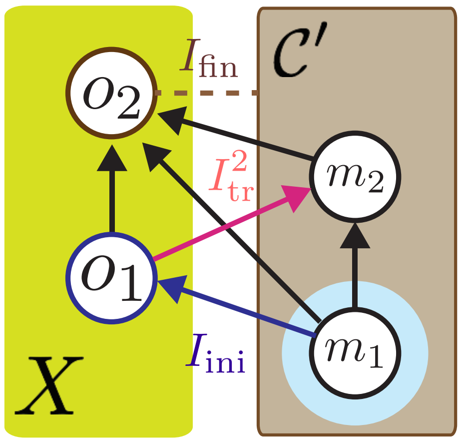

Fig. 6.10 The generalized second law in O on the causal network corresponding to the coupled chemical reaction model with a time-delayed feedback loop.

On the causal network corresponding to this model, we have $i_{\mathrm{fin}} = i(o_2 : \{m_1, m_2\})$, $i_{\mathrm{ini}} = i(o_1 : m_1)$, $i^1_{\mathrm{tr}} = 0$ and $i^2_{\mathrm{tr}} = i(o_1 : m_2|m_1)$ (see also Fig. 6.10). Informational quantity Θ is calculated as

$$\begin{aligned}\Theta &= i(o_2 : \{m_1, m_2\}) - i(o_1 : m_1) - i(o_1 : m_2 | m_1) && (6.103)\\ &= i(o_2 : \{m_1, m_2\}) - i(o_1 : \{m_1, m_2\}) && (6.104)\\ &= \ln p(o_1) - \ln p(o_2) + \ln p(o_2, m_1, m_2) - \ln p(o_1, m_1, m_2) && (6.105)\end{aligned}$$

From the generalized second law Eq.(6.41), we have the following relation

$$-\langle \beta^O \Delta F^O \rangle \geq \langle \ln p(o_2, m_1, m_2) \rangle - \langle \ln p(o_1, m_1, m_2) \rangle. \tag{6.106}$$

The right hand side of Eq. (6.106) is the change in the three-body Shannon entropy, not in the two-body Shannon entropy. This three-body Shannon entropy includes the states of different times m_1 and m_2. This is a crucial difference between the conventional thermodynamics and our general result. Our general result is applicable to non-Markovian dynamics such as the time-delayed feedback loop, where the conventional second law is not valid. In our general result, the Shannon entropy includes the state of different times plays a important role of the generalized second law for non-Markovian dynamics.

Here we numerically illustrate the validity of Eq. (6.106) in Fig. 6.11. In this model, the equilibrium distribution is numerically calculated as $p^O_{0,\mathrm{eq}}(m_1 = 0, m_2 = 0) = 0.332$, $p^O_{0,\mathrm{eq}}(m_1 = 0, m_2 = 1) = 0.310$, $p^O_{0,\mathrm{eq}}(m_1 = 1, m_2 = 0) = 0.289$, and $p^O_{0,\mathrm{eq}}(m_1 = 1, m_2 = 0) = 0.278$. We note that the value of $\langle \sigma \rangle - \langle \Theta \rangle$ in Fig. 6.11 is close to 0 when the initial states are close to the equilibrium distribution of the output system, which is similar to the probability $p^O_{0,\mathrm{eq}}(m_1, m_2)$.

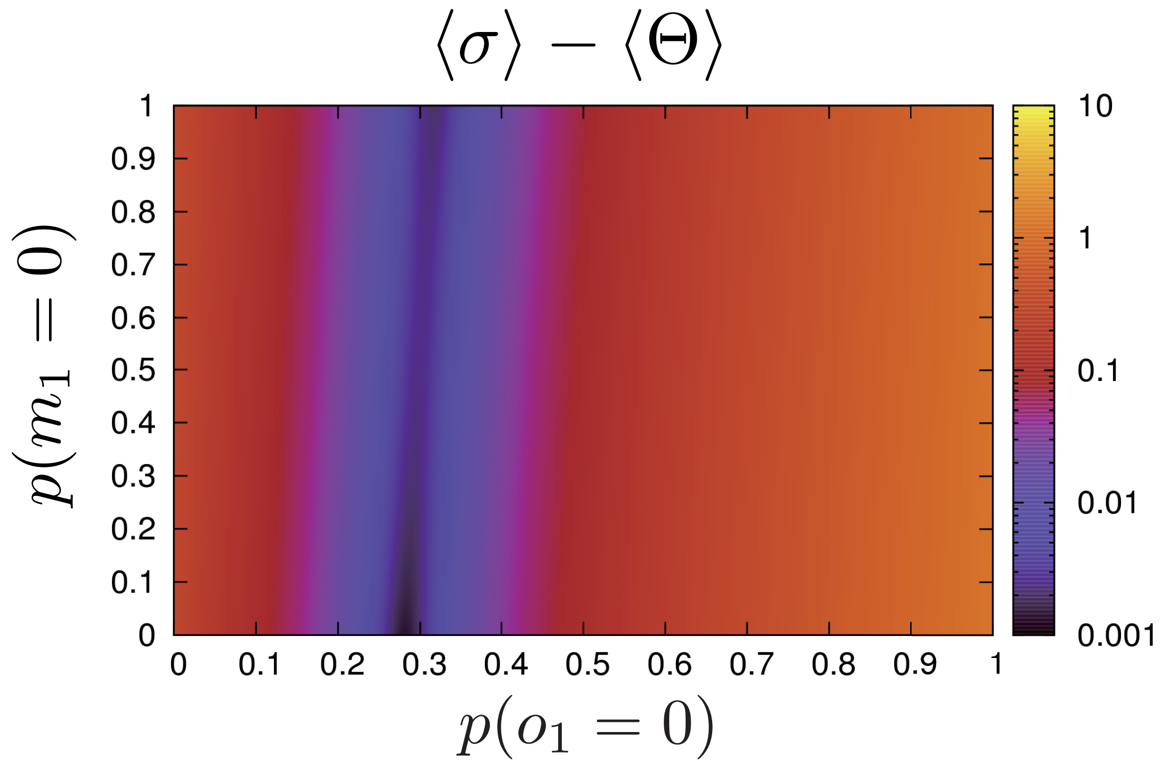

Fig. 6.11 Numerical illustration of the nonnegativity of $\langle\sigma\rangle - \langle\Theta\rangle = -\langle\beta^O \Delta F^O\rangle + \langle\ln p(o_1, m_1, m_2)\rangle - \langle\ln p(o_2, m_1, m_2)\rangle$. We here assume that o_1 and m_1 are independent, i.e., $p(o_1, m_1) = p(o_1)p(m_1)$. We set the parameters as follows: $\Delta t = 0.5$, $\beta^O = \beta^O = 0.01$, $\tau^O = \tau^M = 0.001$, $D^O_{01} = D^M_{01} = 100$, $F^M_0(x_1 = 0) = F^M_0(x_1 = 1) = 100$, $F^M_1(x_1 = 0) = 10$, $F^M_1(x_1 = 1) = 30$, $F^O_0(m_1 = 0, m_2 = 0) = F^O_0(m_1 = 1, m_2 = 0) = F^O_0(m_1 = 0, m_2 = 1) = F^O_0(m_1 = 1, m_2 = 1) = 100$, $F^O_1(m_1 = 0, m_2 = 0) = 30$, $F^O_1(m_1 = 1, m_2 = 0) = 10$, $F^O_1(m_1 = 0, m_2 = 1) = 20$, and $F^O_1(m_1 = 1, m_2 = 1) = 5$.

Chapter 7

Application to Biochemical Signal Transduction

In Chapter 6, we showed that our general theory of information thermodynamics on causal networks is applicable to a broad class of nonequilibrium dynamics, such as a feedback controlled system, coupled Brownian particles and a chemical model with time-delayed feedback control. In this Chapter, we discuss an application of our general result to a biochemical signal transduction, and show that information thermodynamic inequality reveals the fundamental limit of the robustness of signal transduction against environmental fluctuations [59]. Our information-thermodynamic approach is applicable to biochemical communication inside cells, where there is not any explicit channel coding in contrast to the case of artificial communication, i.e., the noisy-channel coding theorem. This chapter is the refinement of our paper submitted [Ito S., & Sagawa T., arXiv: 1406. 5810]. [59]

7.1 Biochemical Signal Transduction

A biochemical signal transduction in living cells is vital to maintain life itself, where the information transmission in a highly noisy environment plays a significant role [4, 5]. For example, the ligand activates the receptor on the cell surface, and the ligand binding triggers the biochemical reaction inside the cell to create the response. Here we discuss the sensory adaptation, which is achieved by a biochemical signal transduction with a negative feedback loop [160].

7.1.1 Sensory Adaptation

Sensory adaptation is an example of the biochemical signal transduction which responds to the stimulus change (e.g., a bacterial chemotaxis, an osmotic sensing in yeast, an olfactory sensing in mammalian neurons, and a light sensing in mammalian neurons) [161]. To become suited to the stimulus change, a negative feedback loop plays a crucial role. For example, a bacterial chemotaxis is a simple model organism for sensory adaptation [162], where the concentration of the kinase activity does not depend on the current concentration of the ligand, but depends on the change of the ligand density. Kinase activity activates a flagellar motor to move bacteria toward a direction of the higher ligand density. To detect the change of the ligand density, the current concentration of the ligand is stored in the memory degree of freedom, and a negative feedback is achieved between the memory and the kinase activity. Thus, the various types of adaptive signal transductions characterizes three components, i.e., the ligand input l, the kinase activity a and the memory m [see also Figure 7.1].

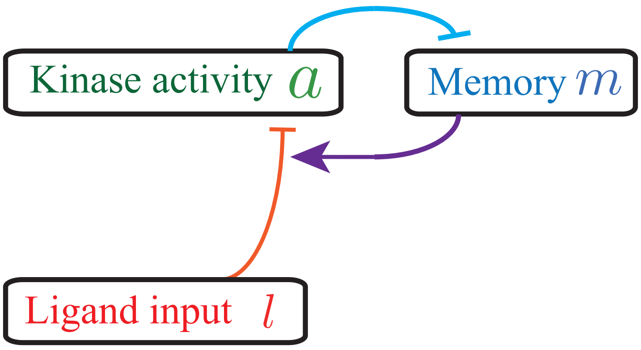

Fig. 7.1 The main components of sensory adaptation are the ligand input l, the kinase activity a and the memory m. The negative feedback loop is in a and m.

We here show the case of *E. coli* (*Escherichia coli*) bacterial chemotaxis in Figure 7.2. The methylation level of the receptor play a role of the memory degree of the freedom m, and restrict the ligand signal l towards the kinase activity a.

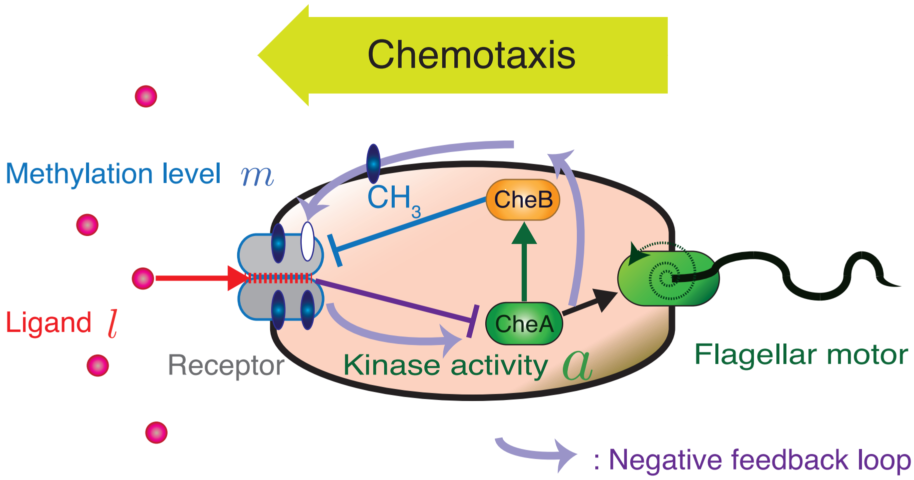

Fig. 7.2 Schematic of the *E. coli* bacterial chemotaxis.

7.1.2 Mutual Information in Biochemical Signal Transduction

Biochemical signaling networks can be highly noisy [163, 164]. To understand the information transmission in noisy environment, the mutual information is a natural measure of information transmission. To address the question how information is transmitted correctly in the presence of noisy biological environment, the mutual information in biochemical signaling networks has been studied theoretically and experimentally. Since the transfer entropy is the conditional mutual information under the condition of the past value, it gives the channel capacity in an artificial communication channel with a feedback loop [see also Figure 7.3]. However, as there is no channel coding inside living cells, the role of the transfer entropy in biological communication is still unclear.

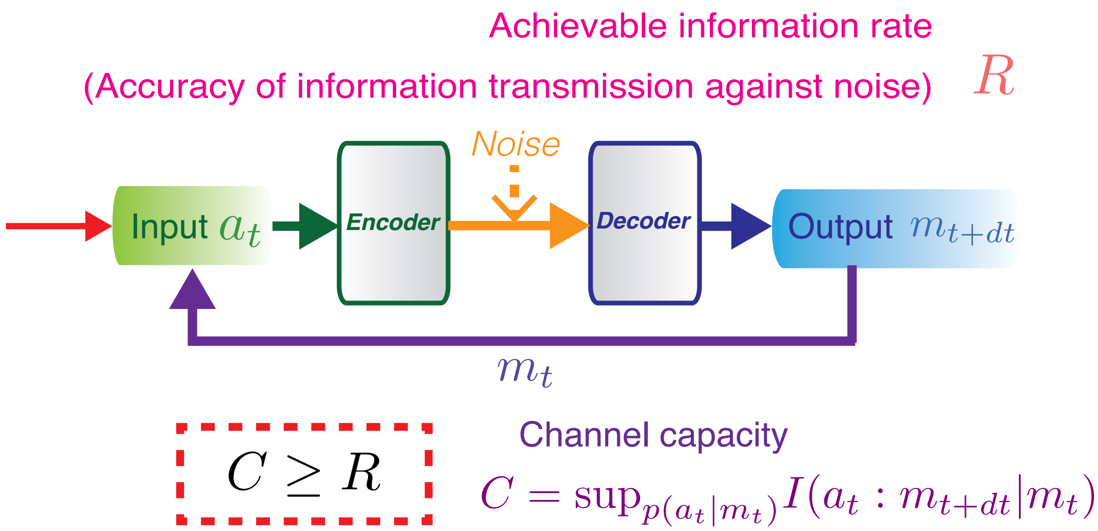

Fig. 7.3 The noisy channel coding theorem in a feedback loop. The transfer entropy $I(a_t : m_{t+dt}|m_t)$ is related to the achievable information rate R in case of a feedback loop.

7.2 Information Thermodynamics in Biochemical Signal Transduction

We here apply our general theory of information thermodynamics for the biochemical signal transduction. To discuss the information-thermodynamic effect in biochemical signal transduction, we analyze the coupled Langevin model of sensory adaptation.

7.2.1 Coupled Langevin Model of Sensory Adaptation

Let a_t be the kinase activity at time t, m_t be the memory degree of freedom (e.g., the methylation level of the receptor in *E. coli* bacterial chemotaxis) at time t, and l_t be the ligand signal at time t. The model of adaptive signal transduction is given by the following coupled Langevin equations [165, 6, 161]:

$$\dot{a}_t = -\frac{1}{\tau^a}[a_t - \bar{a}_t(m_t, l_t)] + \xi^a_t, \tag{7.1}$$

$$\dot{m}_t = -\frac{1}{\tau^m}a_t + \xi^m_t \tag{7.2}$$

where $\bar{a}_t$ is the stationary value of the kinase activity under the instantaneous values of the memory m_t and the ligand signal l_t at time t. ξ_t^x $(x = a, m)$ is the white Gaussian noise at time t with $\langle \xi_t^x \rangle = 0$ and $\langle \xi_t^x \xi_{t'}^{x'} \rangle = 2T_t^x \delta_{xx'} \delta(t-t')$. T_t^x describes the intensity of the environmental noise at time t, which is not necessarily thermal inside cells. The time constants satisfy $\tau^m \gg \tau^a > 0$, which implies that the relaxation of a to $\bar{a}_t$ is much faster than that of m.

In the case of *E. coli* chemotaxis, the stationary value of the kinase activity $\bar{a}_t(m_t, l_t)$ is given by the Monod-Wyman-Changeux allosteric model, which describes the effects of the receptor cooperativity on kinase activity. The Monod-Wyman-Changeux allosteric model [4] is given by the equilibrium distribution of the receptor such as

$$\bar{a}_t(m_t, l_t) = \frac{\exp[-\Delta F(m_t, l_t)]}{1 + \exp[-\Delta F(m_t, l_t)]}, \tag{7.3}$$

where ΔF is the free energy difference between the active and inactive state of the receptor. The free energy difference $\Delta F(m_t, l_t)$ is given by

$$\Delta F(m_t, l_t) = NF_m(\bar{m} - m_t) + N \ln \frac{1 + l_t/K_I}{1 + l_t/K_A}, \tag{7.4}$$

where N is the number of coupled receptor dimers, F_m is a linear constant of free energy of the methylation level, $\bar{m}$ is the methylation value in zero ligand binding, K_I is the dissociation constant corresponding to the inactive state of the receptor, and K_A is the dissociation constant corresponding to the active state of the receptor. In the case of *E. coli* chemotaxis, the dissociation constants satisfy $K_A \gg K_I$. When the stimulus variation of the ligand is within the most sensitive regime of the sensory system (i.e., $K_A \gg l_t \gg K_I$), we can approximate $\bar{a}_t$ as

$$\bar{a}_t(m_t, l_t) = \alpha_m m_t - \alpha_l l_t \tag{7.5}$$

by linearizing it around the steady-state value. Because the ligand signal l_t only appears in the stochastic differential equation of a_t, the noise intensity T_t^a characterizes the ligand fluctuations.

Here we explain the mechanism of sensory adaptation using the coupled Langevin model Eqs. (7.1) and (7.2) [see also Figure 7.4]. Suppose that the system is initially in a stationary state with $a_t = \bar{a}_t(m_t, 0) = 0$ at time $t < 0$, and l_t suddenly changes from 0 to 1 at time $t = 0$ as a step function. Then, a_t rapidly equilibrates to $\bar{a}_t(m_t, 1)$ so that the difference $a_t - \bar{a}_t$ becomes small. Next, m_t gradually changes to $\bar{a}_t(m_t, 1) = 0$ so that a_t returns to 0, where $a_t - \bar{a}_t$ remains small.

7.2.2 Information Thermodynamics and Robustness of Adaptation

We now consider the generalized second law of information thermodynamics for coupled Langevin equations Eqs. (7.1) and (7.2), which can be obtained from Eq. (6.61):

$$dI_t^{\mathrm{tr}} - dI_t^{\mathrm{Btr}} + dS_t^{a|m} \geq \frac{J_t^a}{T_t^a} dt, \tag{7.6}$$

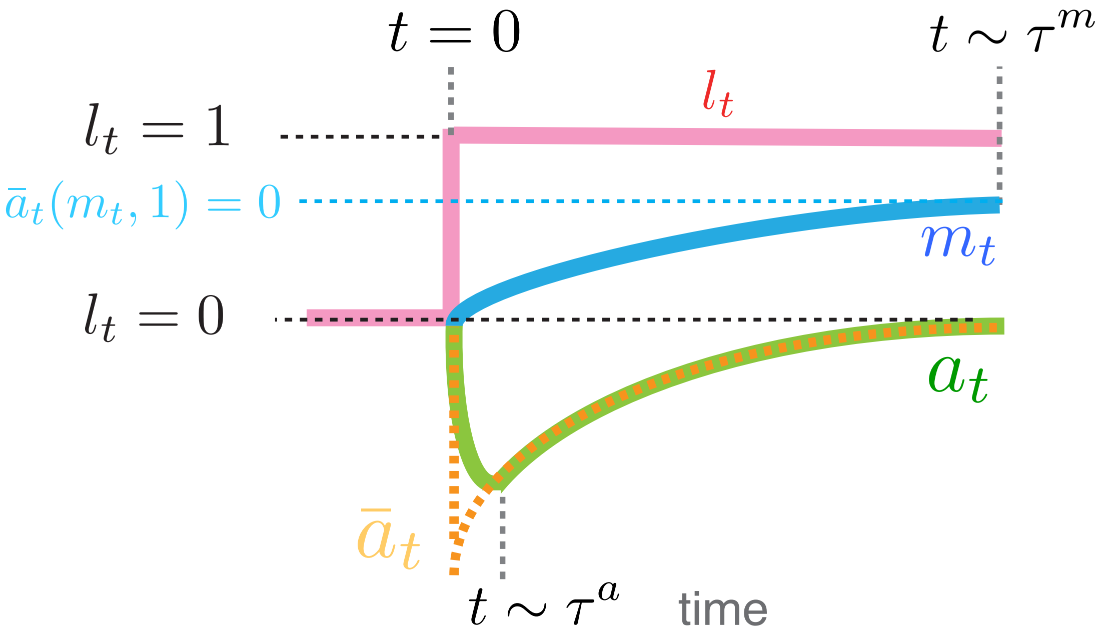

Fig. 7.4 Typical dynamics of adaptation with the ensemble average. Suppose that l_t changes as a step function (red solid line). Then, a_t suddenly responds (green solid line), followed by the gradual response of m_t (blue solid line). The adaptation is achieved by the relaxation of a_t to $\bar{a}_t$ (orange dashed line). The methylation level m_t gradually changes to $\bar{a}_t(m_t, 1) = 0$ (blue dashed line).

where $dI_t^{\rm tr}$ is the transfer entropy defined as $dI_t^{\rm tr} := I(a_t : m_{t+dt}|m_t)$, $dI_t^{\rm Btr}$ is the transfer entropy defined as $dI_t^{\rm Btr} := I(a_{t+dt} : m_t|m_{t+dt})$, $dS_t^{a|m}$ is the conditional Shannon entropy change defined as $dS_t^{a|m} = \langle \ln p(a_t|m_t)\rangle - \langle \ln p(a_{t+dt}|m_{t+dt})\rangle$, and J_t^a is defined as $J_t^a := \langle \dot{a} \circ [\xi_t^a - \dot{a}_t]\rangle$. In the case of the coupled Brownian particles, J_t^a corresponds to the heat absorption in a. Since the environmental noise is not necessarily thermal in the present situation, J_t^a is not exactly the same as the heat absorption. To clarify the role of the transfer entropy $dI_t^{\rm tr}$, we consider the weaker bound of J_t^a as

$$\frac{J_t^a}{T_t^a} dt \leq dI_t^{\rm tr} - dI_t^{\rm Btr} + dS_t^{a|m} \tag{7.7}$$

$$\leq dI_t^{\rm tr} + dS_t^{a|m}, \tag{7.8}$$

where we used the nonnegativity of the conditional mutual information $dI_t^{\rm Btr} \geq 0$. In a stationary state, the conditional Shannon entropy change vanishes (i.e., $dS_t^{a|m}$), and thus the transfer entropy gives the upper bound of J_t^a in a stationary state, i.e., $dI_t^{\rm tr} \geq (J_t^a dt)/T_t^a$.

Here we discuss the biophysical meaning of the quantity J_t^a. The quantity J_t^a can be rewritten by the violation of the fluctuation-dissipation theorem as

$$J_t^a = \langle [\xi_t^a - \dot{a}_t] \circ \dot{a}_t \rangle \tag{7.9}$$

$$= \frac{1}{\tau^a}\left[\langle [a_t - \bar{a}_t] \circ \xi_t^a \rangle - \frac{1}{\tau^a}\langle (a_t - \bar{a}_t)^2 \rangle \right] \tag{7.10}$$

$$= \frac{1}{\tau^a}\left[T_t^a - \frac{1}{\tau^a}\langle (a_t - \bar{a}_t)^2 \rangle \right], \tag{7.11}$$

where we used the relation of the Stratonovich integral $\langle g(a_t, m_t, l_t) \circ \xi_t^a \rangle = T_t^a \langle \partial_{a_t} g(a_t, m_t, l_t) \rangle$ for any function g. This quantity represents the difference between the intensity of the ligand noise T_t^a and the mean square error of the degree of the signal transduction $\langle (a_t - \bar{a}_t)^2 \rangle$. Thus, the quantity J_t^a characterizes the robustness of adaptation against environmental noise. The larger J_t^a is, the more robust the signal transduction is against the environmental noise.

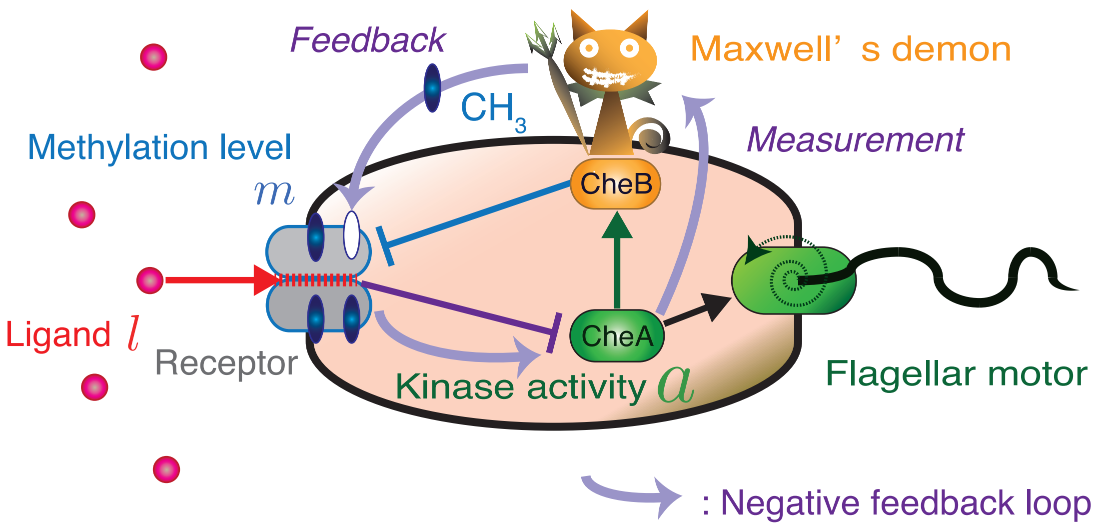

Fig. 7.5 Maxwell's demon in *E. coli* chemotaxis. From the viewpoint of thermodynamics, the methylation level m plays a similar role to the memory of Maxwell's demon, which reduces the effect of the environmental noise on the kinase activity.

To clarify the central idea of our study, we focus on the case of stationary state. If there was no feedback between a and m, information thermodynamics Eq. (7.8) would reduce to

$$\langle (a_t - \bar{a}_t)^2 \rangle \geq \tau^a T_t^a, \tag{7.12}$$

which, as naturally expected, implies that the fluctuation of the signal transduction is bounded by the intensity of the environmental noise. In contrast, in the presence of a feedback loop, information thermodynamics Eq. (7.8) indicates that $\langle (a_t - \bar{a}_t)^2 \rangle$

can be smaller than $\tau^a T_t^a$, owing to the transfer entropy $dI_t^{\rm tr}$ in the feedback loop,

$$\langle (a_t - \bar{a}_t)^2 \rangle \geq \tau^a T_t^a \left[1 - \frac{dI_t^{\rm tr}}{dt} \tau^a \right]. \tag{7.13}$$

This is analogous to the central feature of Maxwell's demon, which implies that information transfer in the feedback loop reduces the effect of the environmental noise on the target system (see also Figure 7.5). This inequality reveals the role of the transfer entropy in biochemical signal transduction; the transfer entropy characterizes the lower bound of the accuracy of the signal transduction in the biochemical network. We add that Yuhai Tu had discussed Maxwell's demon in a biological switch in a different context in 2007 [166].

7.2.3 Information Thermodynamics and Conventional Thermordynamics

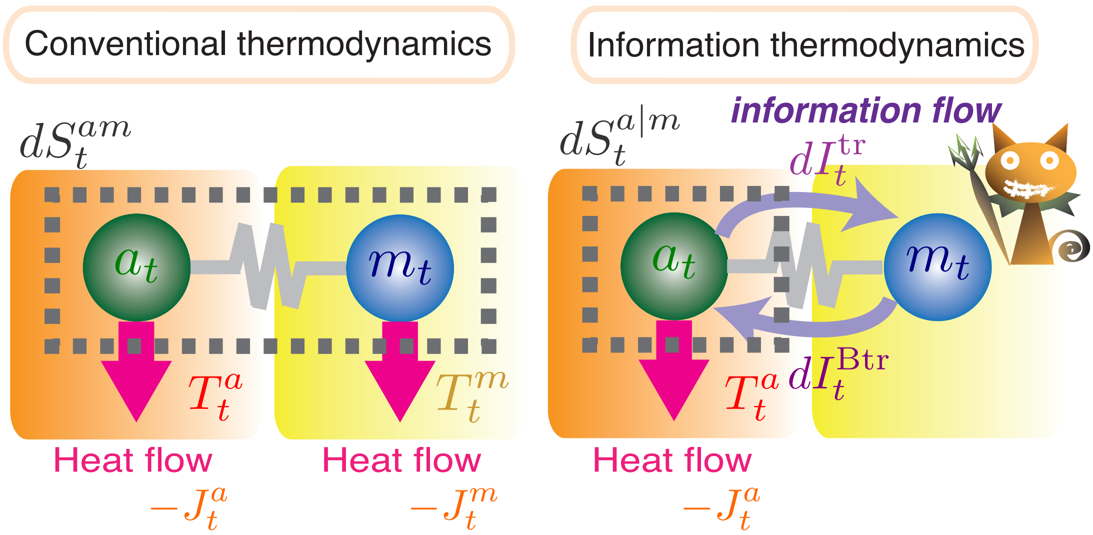

Fig. 7.6 Information thermodynamics and conventional thermodynamics. The second law of information thermodynamics characterizes the entropy change in a subsystem in terms of the information flow between the subsystem and the outside world (i.e., $dI_t^{\rm tr} + dS_t^{a|m} \geq dI_t^{\rm tr} - dI_t^{\rm Btr} + dS_t^{a|m} \geq -J_t^a dt/T_t^a$). In contrast, the conventional second law of thermodynamics states that the entropy change in a subsystem is compensated for by the entropy change in the outside world (i.e., $-J_t^m dt/T_t^m + dS_t^{am} \geq J_t^a dt/T_t^a$).

We next compare the conventional thermodynamics with information thermodynamics. The conventional second law for total systems a and m is given by

$$dS_t^{am} \geq \frac{J_t^a}{T_t^a} dt + \frac{J_t^m}{T_t^m} dt, \tag{7.14}$$

where dS_t^{am} is the total Shannon entropy difference defined as $dS_t^{am} := \langle \ln p(a_t, m_t) \rangle - \langle \ln p(a_{t+dt}, m_{t+dt}) \rangle$, which also vanishes in a stationary state, and J_t^m is the heat absorption in m defined as $J_t^m := \langle \dot{m} \circ [\xi_t^m - \dot{m}_t] \rangle = -\langle a_t^2 \rangle / (\tau^m)^2$. In Figure 7.6, we show the comparison between the conventional thermodynamics and information thermodynamics. In a stationary state, the conventional second law implies that the dissipation in m should compensate for that in a, i.e., $-J_t^m / T_t^m \geq J_t^a / T_t^a$.

We here show numerical comparison between our information thermodynamics and the conventional thermodynamics. We have two upper bounds of the robustness J_t^a, which are given by information thermodynamics and the conventional thermodynamics. Let $\Xi_t^{\rm info} := dI_t^{\rm tr} + dS_t^{a|m}$ be the upper bound of $J_t^a dt / T_t^a$, which is given by the information thermodynamic inequality Eq. (7.8). Let $\Xi_t^{\rm SL} := -J_t^m dt / T_t^m + dS_t^{am}$ be the upper bound of $J_t^a dt / T_t^a$, which is straightforwardly obtained from the conventional second law of thermodynamics Eq. (7.14). Figure 7.7 shows $J_t^a dt / T_t^a$, $\Xi^{\rm info}$ and $\Xi^{\rm SL}$ in six different types of dynamics of adaptation, where the ligand signal and noise are given by step functions (Figure 7.7a), sinusoidal functions (Figure 7.7b), linear functions (Figure 7.7c), exponential decays (Figure 7.7d), square waves (Figure 7.7e) and triangle waves (Figure 7.7f). These results confirm that $\Xi^{\rm info}$ gives a tight bound of J_t^a, implying that the transfer entropy characterizes the robustness well. Remarkably, information thermodynamic bound $\Xi^{\rm info}$ gives a tighter bound of J_t^a than the conventional thermodynamic bound $\Xi_t^{\rm SL}$ such that $\Xi_t^{\rm SL} \geq \Xi_t^{\rm Info} \geq J_t^a dt / T_t^a$ for every non-stationary dynamics shown in Figure 7.7. This fact indicates that the signal transduction of *E. coli* chemotaxis is highly dissipative as a thermodynamic engine, but efficient as an information transmission device.

7.2.4 Analytical Calculations

In the case of *E. coli* chemotaxis, we have $\bar{a}_t = \alpha_m m_t - \alpha_l l_t$ and the coupled Langevin equations Eqs. (7.1) and (7.2) become linear. In this situation, if the initial distribution is Gaussian, we can analytically obtain the transfer entropy up to the order of dt, and compare the information-thermodynamic bound $\Xi^{\rm Info}$ with the conventional thermodynamic bound $\Xi^{\rm SL}$ analytically.

We here generally derive an analytical expression of the transfer entropy for the coupled linear Langevin system:

$$
\begin{aligned}
\dot{x}_t^1 &= \sum_j \mu_t^{1j} x_t^j + f_t^1 + \xi_t^1, \\
\dot{x}_t^2 &= \sum_j \mu_t^{2j} x_t^j + f_t^2 + \xi_t^2, \\
\langle \xi_t^i \xi_{t'}^j \rangle &= 2 T_t^i \delta_{ij} \delta(t - t') \\
\langle \xi_t^i \rangle &= 0,
\end{aligned}
\tag{7.15}
$$

where $i, j = 1, 2$, f_t^i and μ_t^{ij} are time-dependent constants, T_t^i is the time-dependent variance of the white Gaussian noise ξ_t^i, and $\langle \dots \rangle$ denotes the ensemble average. The model of the *E. coli* bacterial chemotaxis is given by Eqs. (6.61) with $\bar{a}_t = \alpha_m m_t - \alpha_l l_t$. To compare the notations of Eqs. (8.16), we set $\{x_t^1, x_t^2\} = \{a_t, m_t\}$, $\mu_t^{11} = -1/\tau^a$, $\mu_t^{12} = \alpha_m / \tau^a$, $f_t^1 = -\alpha_l l_t / \tau^a$, $\mu_t^{21} = -1/\tau^m$, $\mu_t^{22} = 0$, $f_t^2 = 0$, $T_t^1 = T_t^a$, and $T_t^2 = T_t^m$. The transfer entropy from the target system x^1 to the other system x^2 at

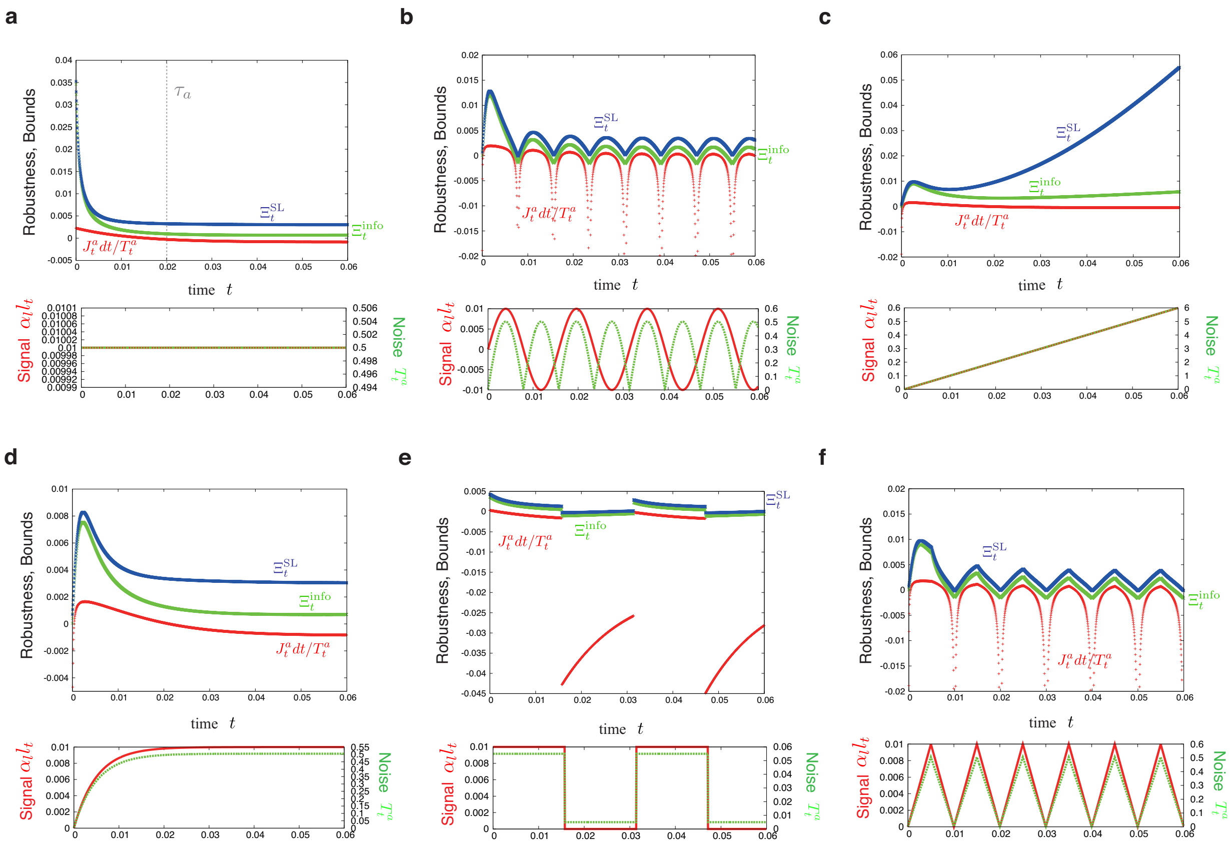

Fig. 7.7 Numerical results of the information thermodynamic bound Ξ^{Info} (green curves) and conventional thermodynamic bound Ξ^{SL} (blue curves) of the robustness $J^a_t dt/T^a_t$ (red curves). The initial condition is the stationary state with $\bar{a}_t = \alpha_m m_t - \alpha_l l_t$, fixed ligand signal $\alpha_l l_t$, and noise intensity $T^a = 0.005$. We numerically confirmed that $\Xi^{\mathrm{SL}}_t \geq \Xi^{\mathrm{Info}}_t \geq J^a_t dt/T^a_t$ holds for the six transition processes. These results imply that, for the signal transduction model, the information-thermodynamic bound is always tighter than the conventional thermodynamic bound. The parameters are chosen as $\tau^a = 0.02$, $\tau^m = 0.2$, $\alpha_m = 2.7$, and $T^m_t = 0.005$, to be consistent with the real parameters of *E. coli* bacterial chemotaxis [165, 161, 6]. **a**, Step function: $\alpha_l l_t = 0.01$ and $T^a_t = 0.5$ for $t > 0$. **b**, Sinusoidal function: $\alpha_l l_t = 0.01 \sin(400t)$ and $T^a_t = 0.5|\sin(400t)| + 0.005$ for $t > 0$. **c**, Linear function: $\alpha_l l_t = 10t$ and $T^a_t = 100t + 0.005$ for $t > 0$. **d**, Exponential decay: $\alpha_l L_t = 0.01[1 - \exp(-200t)]$ and $T^a_t = 0.5[1 - \exp(-200t)] + 0.005$ for $t > 0$. **e**, Square wave: $\alpha_l l_t = 0.01[1 + \lfloor \sin(200t) \rfloor]$ and $T^a_t = 0.05[1 + \lfloor \sin(200t) \rfloor] + 0.005$ for $t > 0$, where $\lfloor \ldots \rfloor$ denotes the floor function. **f**, Triangle wave: $\alpha_l l_t = 0.01|2(100t - \lfloor 100t + 0.5 \rfloor)|$ and $T^a_t = 0.5|2(100t - \lfloor 100t + 0.5 \rfloor)| + 0.005$ for $t > 0$.

time t is defined as $dI_t^{\mathrm{tr}} := \langle \ln p[x_{t+dt}^2 | x_t^1, x_t^2] \rangle - \langle \ln p[x_{t+dt}^2 | x_t^2] \rangle$.

Here, we analytically calculate the transfer entropy for the case that the joint probability $p[x_t^1, x_t^2]$ is a Gaussian distribution:

$$p[x_t^1, x_t^2] = \frac{1}{(2\pi)\sqrt{\det \Sigma_t}} \exp\left[-\sum_{ij} \frac{1}{2} \bar{x}_t^i G_t^{ij} \bar{x}_t^j \right], \tag{7.16}$$

where Σ_t^{ij} is the covariant matrix $\Sigma_t^{ij} := \langle x_t^i x_t^j \rangle - \langle x_t^i \rangle \langle x_t^j \rangle$, and $\bar{x}_t^j := x_t^j - \langle x_t^j \rangle$. The inverse matrix $G_t := \Sigma_t^{-1}$ satisfies $\sum_j G_t^{ij} \Sigma_t^{jl} = \delta_{il}$ and $G_t^{ij} = G_t^{ji}$. The joint distribution $p[x_t^2]$ is given by the Gaussian probability:

$$p[x_t^2] = \frac{1}{\sqrt{2\pi \Sigma_t^{22}}} \exp\left[-\frac{1}{2} (\Sigma_t^{22})^{-1} (\bar{x}_t^2)^2 \right]. \tag{7.17}$$

We consider the path-integral expression of the Langevin equation (8.16). The conditional probability $p[x_{t+dt}^2 | x_t^1, x_t^2]$ is given by

$$\begin{aligned} p[x_{t+dt}^2 | x_t^1, x_t^2] &= \mathcal{N} \exp\left[-\frac{dt}{4T_t^2} \left(\frac{x_{t+dt}^2 - x_t^2}{dt} - \sum_j \mu_t^{2j} x_t^j - f_t^2 \right)^2 \right] & (7.18) \\ &= \mathcal{N} \exp\left[-\frac{dt}{4T_t^2} \left(F_t^2 - \mu_t^{21} \bar{x}_t^1 \right)^2 \right], & (7.19) \end{aligned}$$

where $\mathcal{N}$ is the normalization constant with $\int dx_{t+dt}^2 p[x_{t+dt}^2 | x_t^1, x_t^2] = 1$. For the simplicity of notation, we set $F_t^2 = (x_{t+dt}^2 - x_t^2)/dt - \mu_t^{21} \langle x_t^1 \rangle - \mu_t^{22} x_t^2 - f_t^2$. From Eqs. (8.17) and (8.19), we have the joint distribution $p[x_{t+dt}^2, x_t^2]$ as

$$\begin{aligned} p[x_{t+dt}^2, x_t^2] &= \int dx_t^1 p[x_{t+dt}^2 | x_t^1, x_t^2] p[x_t^1, x_t^2] \\ &= \frac{\mathcal{N}}{\sqrt{4\pi \det \Sigma_t \left(\frac{dt}{4T_t^2} (\mu_t^{21})^2 + \frac{G_t^{11}}{2} \right)}} \\ &\quad \times \exp\left[-\frac{dt}{4T_t^2} (F_t^2)^2 - \frac{1}{2} G_t^{22} (\bar{x}_t^2)^2 + \frac{\left(G_t^{12} \bar{x}_t^2 - \frac{\mu_t^{21} F_t^2}{2T_t^2} dt \right)^2}{4 \left(\frac{dt}{4T_t^2} (\mu_t^{21})^2 + \frac{G_t^{11}}{2} \right)} \right]. \end{aligned} \tag{7.20}$$

From Eqs. (8.18), (8.19), and (8.20), we obtain the analytical expression of the transfer entropy $dI_t^{\rm tr}$ up to the order of dt:

$$
\begin{aligned}
dI_t^{\rm tr} :=& \langle \ln p[x^2_{t+dt}|x^2_t, x^1_t] + \ln p[x^2_t] - \ln p[x^2_{t+dt}, x^2_t] \rangle \\
=& -\frac{dt}{4T_t^2}\langle \left(F_t^2 - \mu_t^{21}\bar{x}_t^1\right)^2 \rangle - \frac{1}{2}\ln\left[2\pi\Sigma_t^{22}\right] - \frac{1}{2}(\Sigma_t^{22})^{-1}\langle(\bar{x}_t^2)^2\rangle \\
&+ \frac{1}{2}\ln\left[4\pi\det\Sigma_t\left(\frac{dt}{4T_t^2}(\mu_t^{21})^2 + \frac{G_t^{11}}{2}\right)\right] \\
&+ \frac{dt}{4T_t^2}\langle(F_t^2)^2\rangle + \frac{1}{2}G_t^{22}\langle(\bar{x}_t^2)^2\rangle - \frac{\left\langle\left(G_t^{12}\bar{x}_t^2 - \frac{\mu_t^{21}F_t^2}{2T_t^2}dt\right)^2\right\rangle}{4\left(\frac{dt}{4T_t^2}(\mu_t^{21})^2 + \frac{G_t^{11}}{2}\right)} \\
=& \frac{\mu^{21}dt}{2T_t^2}\langle F_t^2\bar{x}_t^1\rangle - \frac{dt}{4T_t^2}(\mu_t^{21})^2\Sigma_t^{11} - \frac{1}{2} + \frac{(\mu_t^{21})^2 dt}{4G_t^{11}T_t^2} + \frac{1}{2}G_t^{22}\Sigma_t^{22} \\
&- \frac{(G_t^{12})^2\Sigma_t^{22}}{2G_t^{11}}\left[1 - \frac{dt}{2G_t^{11}T_t^2}(\mu_t^{21})^2\right] + \frac{\mu_t^{21}dt}{2G_t^{11}T_t^2}G_t^{12}\langle F_t^2\bar{x}_t^2\rangle - \frac{(\mu_t^{21})^2 dt}{4G_t^{11}T_t^2} + \mathcal{O}(dt^2) \\
=& \frac{\mu^{21}dt}{2T_t^2}\langle F_t^2\bar{x}_t^1\rangle + \frac{\mu_t^{21}dt}{2G_t^{11}T_t^2}G_t^{12}\langle F_t^2\bar{x}_t^2\rangle - \frac{(\mu_t^{21})^2 dt}{4G_t^{11}T_t^2} + \mathcal{O}(dt^2) \\
=& \frac{(\mu_t^{21})^2}{4T_t^2}\frac{\det\Sigma_t}{\Sigma_t^{22}}dt + \mathcal{O}(dt^2) \\
=& \frac{1}{2}\ln\left(1 + \frac{dP_t}{N_t}\right) + \mathcal{O}(dt^2),
\end{aligned}
\tag{7.21}
$$

where we define $dP_t := (\mu_t^{21})^2(\det\Sigma_t)dt/(\Sigma_t^{22})$, and $N_t := 2T_t^2$. In this calculation, we used $G_t^{ij} = G_t^{ji}$, $\Sigma_t^{ij} = \Sigma_t^{ji}$, $G_t^{i1}\Sigma_t^{1l} + G_t^{i2}\Sigma_t^{2l} = \delta_{ij}$, $\langle(F_t^2)^2\rangle dt^2 = 2T_t^2 dt + \mathcal{O}(dt^2)$, $\langle F_t^2\bar{x}_t^1\rangle = \mu_t^{21}\Sigma_t^{11}$, $\langle F_t^2\bar{x}_t^2\rangle = \mu_t^{21}\Sigma_t^{12}$, and $G_t^{11} = (\Sigma_t^{22})/(\det\Sigma_t)$.

In the model of the *E. coli* bacterial chemotaxis, we have $N_t = 2T_t^m$ and

$$
\begin{aligned}
dP_t &= \frac{1}{(\tau^m)^2}\frac{[\langle a_t^2\rangle - \langle a_t\rangle^2][\langle m_t^2\rangle - \langle m_t\rangle^2] - [\langle a_t m_t\rangle - \langle a_t\rangle\langle m_t\rangle]^2}{\langle m_t^2\rangle - \langle m_t\rangle^2}dt \\
&= \frac{1-(\rho_t^{am})^2}{(\tau^m)^2}V_t^a dt,
\end{aligned}
\tag{7.22}
$$

where $V_t^x := \langle x_t^2\rangle - \langle x_t\rangle^2$ indicates the variance of $x_t = a_t$ or $x_t = m_t$, and $\rho_t^{am} := [\langle a_t m_t\rangle - \langle a_t\rangle\langle m_t\rangle]/(V_t^a V_t^m)^{1/2}$ is the correlation coefficient of a_t and m_t. The correlation coefficient ρ_t^{am} satisfies $-1 \leq \rho_t^{am} \leq 1$, because of the Cauchy-Schwartz inequality. We note that, if the joint probability $p(a_t, m_t)$ is Gaussian, the factor $1 - (\rho_t^{am})^2$ can be rewritten by the mutual information I_t^{am} as

$$
1 - (\rho_t^{am})^2 = \exp[-2I_t^{am}], \tag{7.23}
$$

where I_t^{am} is defined as $I_t^{am} := \int da_t dm_t p[a_t, m_t]\ln[p[a_t, m_t]/[p[a_t]p[m_t]]]$. This fact implies that, if the target system a_t and the other system m_t are strongly correlated (i.e., $I_t^{am} \to \infty$), no information flow exists (i.e., $dI_t^{\rm tr} \to 0$).

From the analytical expression of the transfer entropy Eq. (7.21), we can analytically compare the conventional thermodynamic bound (i.e., $\Xi_t^{\mathrm{SL}} := -J_t^m dt/T_t^m + dS_t^{am} \geq J_t^a dt/T_t^a$) with the information-thermodynamic bound (i.e., $\Xi_t^{\mathrm{Info}} = dI_t^{\mathrm{tr}} + dS_t^{a|m} \geq J_t^a dt/T_t^a$) for the model of *E. coli* chemotaxis [Eqs. (7.1) and (7.2) with $\bar{a}_t = \alpha m_t - \beta l_t$] in a stationary state, where both of the Shannon entropy and the conditional Shannon changes vanish, i.e., $dS_t^{a|m} = 0$ and $dS_t^{am} = 0$. Thus, the conventional thermodynamic bound is given by the heat emission from m such that $\Xi_t^{\mathrm{SL}} = -J_t^m dt/T_t^m$, and the information thermodynamic bound is given by the information flow such that $\Xi_t^{\mathrm{Info}} = dI_t^{\mathrm{tr}}$. The information thermodynamic bound is given by $\Xi_t^{\mathrm{Info}} = (1-(\rho_t^{am})^2)[\langle a_t^2\rangle - \langle a_t\rangle^2]dt/[2(\tau^m)^2 T_t^m]$. The conventional thermodynamic bound is given by $\Xi_t^{\mathrm{SL}} = \langle a_t^2\rangle dt/[(\tau^m)^2 T_t^m]$. From $-1 \leq \rho_t^{am} \leq 1$ and $\langle a_t\rangle^2 \geq 0$, we have the inequality $\Xi_t^{\mathrm{SL}} \geq \Xi_t^{\mathrm{Info}}$. This implies that the information-thermodynamic bound Ξ_t^{Info} is tighter than the conventional bound Ξ_t^{SL} for the model of *E. coli* bacterial chemotaxis:

$$\Xi_t^{\mathrm{SL}} \geq \Xi_t^{\mathrm{Info}} \geq J_t^a dt/T_t^a. \tag{7.24}$$

7.3 Information Thermodynamics and Noisy-Channel Coding Theorem

We discuss the similarity and the difference between our result and Shannon's noisy channel coding theorem.

7.3.1 Analogical Similarity

The noisy channel coding theorem states that the upper bound of archivable information rate R is given by the channel capacity C. The channel capacity C is defined as the supremum value of mutual information between input and output with a finite input power. The mutual information can be replaced by the transfer entropy dI_t^{tr} in the presence of a feedback loop. R describes how long bit sequence is needed for a channel coding, to realize errorless communication through a noisy channel. where errorless means the coincidence between the input and output messages. On the other hand, information thermodynamics states that the robustness of the biochemical signal transduction J_t^a is bounded by the transfer entropy dI_t^{tr}. Therefore both of J_t^a and R characterize the robust information transmission against noise and are bounded by the transfer entropy dI_t^{tr}. In this sense, there exists an analogy between the second law of thermodynamics with information and the noisy channel coding theorem, in spite of the fact that they are very different in general (see also Fig. 7.8).

7.3.2 Difference and Biochemical Relevance

In general, the archivable rate R is different from the robustness J_t^a. In the case of biochemical signal transduction, information thermodynamic approach is more relevant, because there is not any explicit channel coding inside cells. Moreover,

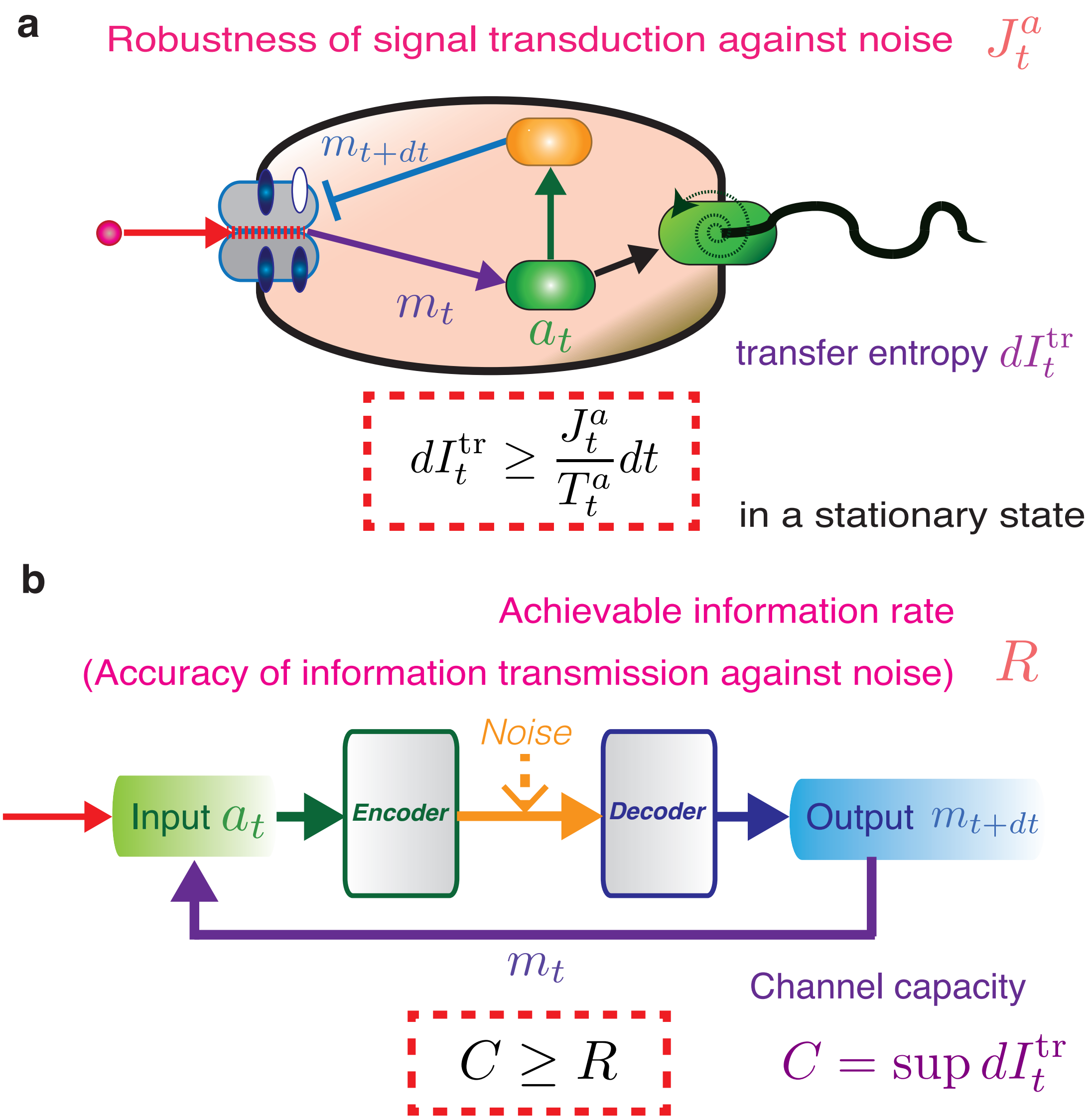

Fig. 7.8 Analogy and difference between our approach and Shannon's noisy channel coding theorem. **a**, Information thermodynamics for biochemical signal transduction. The robustness J_t^a is bounded by the information flow dI_t^{tr} in stationary states, which is a consequence of the second law of information thermodynamics. **b**, Information theory for artificial communication. The archivable information rate R, given by the redundancy of the channel coding, is bounded by the channel capacity $C = \max dI_t^{\mathrm{tr}}$, which is a consequence of the Shannon's second theorem. If the noise is Gaussian as is the case for *E. coli* chemotaxis, both of the transfer entropy and the channel capacity are given by the power-to-noise ratio $C = dI_t^{\mathrm{tr}} = (2)^{-1} \ln(1 + dP_t/N_t)$, under the condition that the initial distribution is Gaussian.

while J_t^a is an experimentally measurable quantity [72, 74], R cannot be properly defined without any artificial channel coding [2]. Therefore, J_t^a is an intrinsic quantity to characterize the accuracy of the information transduction inside cells without any artificial channel coding process. From the information thermodynamic point of view, we can discuss the efficiency of information without any assumption of the channel coding inside cells. We can also discuss the thermodynamic efficiency as a heat engine in parallel.

Chapter 8

Information Thermodynamics as Stochastic Thermodynamics for Small Subsystem

In this chapter, we first focus on information thermodynamics for a multi-dimensional Markov process. We will show that information thermodynamics can be considered as the stochastic thermodynamics for small subsystems. From a thermodynamic point of view, the backward transfer entropy plays an important role as the conventional transfer entropy. We next generalize information thermodynamics on causal networks using the backward transfer entropy. Our generalization gives a tighter lower bound of the entropy production in a subsystem.

8.1 Information Thermodynamics for Small Subsystem

In Chapter 6, we have given the general formalism of information thermodynamics for two-dimensional Langevin system. We here focus on the case of a multi-dimensional Markov process.

8.1.1 Information thermodynamics for a multi-dimensional Markov process

We consider a situation that dynamics of multi-dimensional system $\{X^1, \ldots, X^{n_{\rm sys}})\}$ is Markovian, where $n_{\rm sys}$ is a number of small fluctuating systems. Let the path of a small subsystem X^i be $X^i = \{x^i_k | k = 0, 1, \ldots, N\}$, and the path of the other system be $\boldsymbol{X}^{-i} = \{\boldsymbol{x}^{-i}_k | k = 1, \ldots, N\} = \{x^\nu_k | \nu = 1, \ldots, i-1, i+1, \ldots, n_{\rm sys}, k = 1, \ldots, N\}$, where k denotes time. We assume that the path probability $p(X^i, \boldsymbol{X}^{-i})$ is given by

$$p(X^i, \boldsymbol{X}^{-i}) = p(x^i_1, \boldsymbol{x}^{-i}_1) \prod_{k=1}^{N-1} p(x^i_{k+1} | x^i_k, \boldsymbol{x}^{-i}_k) p(\boldsymbol{x}^{-i}_{k+1} | x^i_k, \boldsymbol{x}^{-i}_k) \tag{8.1}$$

$$= p(x^i_1, \ldots, x^{n_{\rm sys}}_1) \prod_{k=1}^{N-1} \prod_{\nu=1}^{n_{\rm sys}} p(x^\nu_{k+1} | x^i_k, \ldots, x^{n_{\rm sys}}_k). \tag{8.2}$$

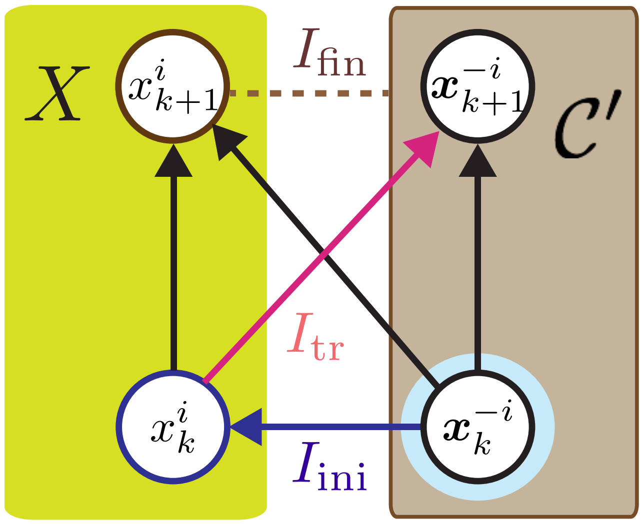

Fig. 8.1 A causal network corresponding to Eq. (8.4).

From the path probability Eq. (8.2), we calculate the joint probability $p(x^i_{k+1}, \boldsymbol{x}^{-i}_{k+1}, x^i_k, \boldsymbol{x}^{-i}_k)$ with $1 \leq k \leq N-1$ as

$$p(x^i_k, \boldsymbol{x}^{-i}_{k+1}, x^i_k, \boldsymbol{x}^{-i}_k) = \sum_{\{X^i, \boldsymbol{X}^{-i}\} \setminus \{x^i_{k+1}, \boldsymbol{x}^{-i}_{k+1}, x^i_k, \boldsymbol{x}^{-i}_k\}} p(X^i, \boldsymbol{X}^{-i}) \tag{8.3}$$

$$= p(x^i_k, \boldsymbol{x}^{-i}_k) p(x^i_{k+1} | x^i_k, \boldsymbol{x}^{-i}_k) p(\boldsymbol{x}^{-i}_{k+1} | x^i_k, \boldsymbol{x}^{-i}_k). \tag{8.4}$$

We next consider a causal network for Eq. (8.4) (see Fig. 8.1). This causal network shows a single time step of the Markovian dynamics from time k to time $k+1$. By the discussion in Chapter 6, the entropy production for a small subsystem X^i is bounded by the information quantity Θ, which is given by the graph Fig. 8.1 as

$$\Theta := i_{\rm fin} - i_{\rm ini} - \sum_{l=1}^{2} i^l_{\rm tr}, \tag{8.5}$$

$$\begin{aligned} i_{\rm ini} &= i(x_1 : {\rm pa}(x_1)) \\ &= i(x^i_k : \boldsymbol{x}^{-i}_k), \end{aligned} \tag{8.6}$$

$$\begin{aligned} i^1_{\rm tr} &= i(c_1 : {\rm pa}_X(c_1)) \\ &= 0, \end{aligned} \tag{8.7}$$

$$\begin{aligned} i^2_{\rm tr} &= i(c_2 : {\rm pa}_X(c_2) | c_1) \\ &= i(x^i_k : \boldsymbol{x}^{-i}_{k+1} | \boldsymbol{x}^{-i}_k), \end{aligned} \tag{8.8}$$

$$\begin{aligned} i_{\rm fin} &= i(x^2 : \mathcal{C}') \\ &= i(x^i_{k+1} : \{\boldsymbol{x}^{-i}_k, \boldsymbol{x}^{-i}_{k+1}\}), \end{aligned} \tag{8.9}$$

where we set $X = \{x_1 = x^i_k, x_2 = x^i_{k+1}\}$, $\mathcal{C} = \mathcal{C}' = \{c_1 = \boldsymbol{x}^{-i}_k, c_2 = \boldsymbol{x}^{-i}_{k+1}\}$, ${\rm pa}(x^i_k) = \boldsymbol{x}^{-i}_k$, ${\rm pa}_X(\boldsymbol{x}^{-i}_k) = \emptyset$, and ${\rm pa}_X(\boldsymbol{x}^{-i}_{k+1}) = x^i_k$.

Let σ^k be the entropy production for the single time step $\sigma^k := \ln p(x^i_k) - \ln p(x^i_{k+1}) + \Delta s^k_{\mathrm{bath}}$, where $\Delta s^k_{\mathrm{bath}}$ is the entropy change in heat baths from time k to $k+1$ by the system X^i. We then have the inequality $\langle \sigma^k \rangle \geq \langle \Theta \rangle$ for each k such as

$$S(x^i_{k+1}) - S(x^i_k) + \langle \Delta s^k_{\mathrm{bath}} \rangle \geq I(x^i_k : \{\boldsymbol{x}^{-i}_k, \boldsymbol{x}^{-i}_{k+1}\}) - I(x^i_{k+1} : \{\boldsymbol{x}^{-i}_k, \boldsymbol{x}^{-i}_{k+1}\}), \quad (8.10)$$

or equivalently

$$S(x^i_{k+1}|\boldsymbol{x}^{-i}_{k+1}) - S(x^i_k|\boldsymbol{x}^{-i}_k) + \langle \Delta s^k_{\mathrm{bath}} \rangle \geq I^{\mathrm{Btr}}_k - I^{\mathrm{tr}}_k, \quad (8.11)$$

where $I^{\mathrm{tr}}_k := I(x^i_k : \boldsymbol{x}^{-i}_{k+1}|\boldsymbol{x}^{-i}_k)$ is the transfer entropy from a small subsystem X^i to the outside worlds $\boldsymbol{X}^{-i}$ at time k and $I^{\mathrm{Btr}}_k := I(x^i_{k+1} : \boldsymbol{x}^{-i}_k|\boldsymbol{x}^{-i}_{k+1})$ is the backward transfer entropy from a small subsystem X^i to the outside worlds $\boldsymbol{X}^{-i}$ at time k. We note that the difference $I^{\mathrm{Btr}}_k - I^{\mathrm{tr}}_k$ gives the net information flow in the dynamics at time k. To sum up Eq. (8.11) with $k = 1, \ldots, N-1$, we have the information thermodynamic inequality for subsystem X^i as

$$\langle \sigma^{i|-i} \rangle \geq \sum_{k=1}^{N-1} I^{\mathrm{Btr}}_k - \sum_{k=1}^{N-1} I^{\mathrm{tr}}_k \quad (8.12)$$

$$\geq - \sum_{k=1}^{N-1} I^{\mathrm{tr}}_k, \quad (8.13)$$

$$(8.14)$$

where $\sigma^{i|-i} := \sum_{k=1}^{N-1} \Delta s^k_{\mathrm{bath}} - \ln p(x^i_N|\boldsymbol{x}^{-i}_N) + \ln p(x^i_1|\boldsymbol{x}^{-i}_1)$ gives the conditional entropy production in a small subsystem X^i.

The sums of the transfer entropy $\sum_{k=1}^{N-1} I^{\mathrm{tr}}_k$ and of the backward transfer entropy $\sum_{k=1}^{N-1} I^{\mathrm{Btr}}_k$ play crucial roles in stochastic thermodynamics for a small subsystem. The conditional entropy production in a small subsystem can be negative, and its lower bound is given by the sum of transfer entropy [i.e., $\langle \sigma^{i|-i} \rangle \geq -\sum_{k=1}^{N-1} I^{\mathrm{tr}}_k$]. This fact implies that the sum of the transfer entropy $\sum_{k=1}^{N-1} I^{\mathrm{tr}}_k$ gives the thermodynamic benefit in a small subsystem X^i. On the other hand, the sum of backward transfer entropy $\sum_{k=1}^{N-1} I^{\mathrm{Btr}}_k$ gives the thermodynamic loss in a small subsystem X^i. The backward transfer entropy $\sum_{k=1}^{N-1} I^{\mathrm{Btr}}_k$ can be considered as the inevitable dissipation in a small subsystem, because Eq. (8.14), which includes the backward transfer entropy, gives a tighter bound of the conditional production compared to the inequality $\langle \sigma^{i|-i} \rangle \geq -\sum_{k=1}^{N-1} I^{\mathrm{tr}}_k$.

We add the continuous case of Eq. (8.14). Let $x^i(t)$ be the state of a small subsystem X^i at continuous time t, and $\boldsymbol{x}^{-i}(t)$ be the states of the outside worlds $\boldsymbol{X}^{-i}$ at continuos time t. In the continuous limit of Eq. (8.14), we have

$$\langle \sigma^{i|-i} \rangle \geq \int_{t=0}^{\tau} dt \frac{dI^{\mathrm{Btr}}_t}{dt} - \int_{t=0}^{\tau} dt \frac{dI^{\mathrm{tr}}_t}{dt}, \quad (8.15)$$

where $\sigma^{i|-i} := \Delta s_{\mathrm{bath}} - \ln p(x^i(\tau)|\boldsymbol{x}^{-i}(\tau)) + \ln p(x^i(0)|\boldsymbol{x}^{-i}(0))$ is the conditional entropy production in a small subsystem with entropy change in heat baths Δs_{bath} by a small subsystem X^i from time $t=0$ to $t=\tau$, $dI_t^{\rm Btr}/dt$ is the backward transfer entropy flow defined as $dI_t^{\rm Btr}/dt := I(x^i(t+dt) : \boldsymbol{x}^{-i}(t)|\boldsymbol{x}^{-i}(t+dt))/dt$, and $dI_t^{\rm tr}/dt$ is the transfer entropy flow defined as $dI_t^{\rm tr}/dt := I(x^i(t) : \boldsymbol{x}^{-i}(t+dt)|\boldsymbol{x}^{-i}(t))/dt$ with an infinitesimal time interval dt.

8.1.2 Transfer Entropy for Multi-Dimensional Linear Langevin System

We here show an analytical expression of the transfer entropy for a multi-dimensional linear Langevin system, which gives a lower bound of the conditional entropy production in a small subsystem X^i, i.e., $\langle \sigma^{i|-i} \rangle \geq -\int_{t=0}^{\tau} dt[dI_t^{\rm tr}/dt]$. We calculate the transfer entropy from one of$n_{\rm sys}$ pieces of variables to the other $n_{\rm sys}-1$ pieces of variables; this calculation is a generalization of Sec. 7.2.4. We here consider the following $n_{\rm sys}$-dimensional linear Langevin equation:

$$\begin{aligned} \dot{x}_t^i &= \sum_j \mu_t^{ij} x_t^j + f_t^i + \xi_t^i, \\ \langle \xi_t^i \xi_{t'}^j \rangle &= 2T_t^i \delta_{ij} \delta(t-t') \\ \langle \xi_t^i \rangle &= 0, \end{aligned} \tag{8.16}$$

where $i,j = 1,\ldots,n_{\rm sys}$. f_t^i and μ_t^{ij} are time-dependent constants at time t. T_t^i is the time-dependent variance of the white Gaussian noise ξ_t^i. $\boldsymbol{x}_t^{-i} := \{x_t^{\nu}|\nu \neq i\}$ is the variables of the other systems $\boldsymbol{X}^{-i}$. The transfer entropy from the target system X^i to the other systems $\boldsymbol{X}^{-i}$ at time t is given by $dI_t^{\rm tr} := \langle \ln p(\boldsymbol{x}_{t+dt}^{-i}|x_t^i, \boldsymbol{x}_t^{-i})\rangle - \langle \ln p(\boldsymbol{x}_{t+dt}^{-i}|\boldsymbol{x}_t^{-i})\rangle$. The covariance matrix is defined as $\Sigma_t^{ij} := \langle x_t^i x_t^j \rangle - \langle x_t^i \rangle \langle x_t^j \rangle$. We assume that the joint probability $p(x_t^i, \boldsymbol{x}_t^{-i})$ is a Gaussian distribution of the form

$$p(x_t^i, \boldsymbol{x}_t^{-i}) = \frac{1}{(2\pi)^{\frac{n_{\rm sys}}{2}} \sqrt{\det \Sigma_t}} \exp\left[-\sum_{ij} \frac{1}{2} \bar{x}_t^i G_t^{ij} \bar{x}_t^j \right], \tag{8.17}$$

where $\bar{x}_t^j := x_t^j - \langle x_t^j \rangle$. The inverse matrix $G_t := \Sigma_t^{-1}$ satisfies $\sum_j G_t^{ij} \Sigma_t^{jl} = \delta_{il}$ and $G_t^{ij} = G_t^{ji}$, where δ_{il} is Kronecker's delta. The joint distribution $p(\boldsymbol{x}_t^{-i})$ is given by the Gaussian probability,

$$\begin{aligned} p(\boldsymbol{x}_t^{-i}) &= \int dx_t^i p(x_t^i, \boldsymbol{x}_t^{-i}) \\ &= \frac{1}{(2\pi)^{\frac{n_{\rm sys}-1}{2}} \sqrt{\det \tilde{\Sigma}_t}} \exp\left[-\sum_{i'j'} \frac{1}{2} \bar{x}_t^{i'} \tilde{G}_t^{i'j'} \bar{x}_t^{j'} \right], \end{aligned} \tag{8.18}$$

where i', j' $(\neq i)$ denote the indexes of the other systems. $\tilde{\Sigma}_t^{i'j'}$ is the covariance matrix which satisfies $\tilde{\Sigma}_t^{i'j'} = \langle x_t^{i'} x_t^{j'} \rangle - \langle x_t^{i'} \rangle \langle x_t^{j'} \rangle$, $\sum_{j'} \tilde{G}_t^{i'j'} \tilde{\Sigma}_t^{j'l'} = \delta_{i'l'}$ and $G_t^{ii} = (\det \tilde{\Sigma}_t)/(\det \Sigma_t)$.

We consider the path-integral expression of the Langevin equation (8.16). The conditional probability $p(\boldsymbol{x}_{t+dt}^{-i}|x_t^i, \boldsymbol{x}_t^{-i})$ is given by

$$p(\boldsymbol{x}_{t+dt}^{-i}|x_t^i, \boldsymbol{x}_t^{-i}) = \mathcal{N} \exp\left[-\sum_{j'} \frac{dt}{4T_t^{j'}} (F_t^{j'} - \mu^{j'i}\bar{x}_t^i)^2 \right], \tag{8.19}$$

where $\mathcal{N}$ is the prefactor, and we set $F_t^{j'} = \mu^{j'i}\bar{x}_t^i + \xi_t^{j'}$. To obtain the analytical expression of the transfer entropy, we calculate the joint probability distribution $p(\boldsymbol{x}_{t+dt}^{-i}, \boldsymbol{x}_t^{-i})$. From Eqs. (8.17) and (8.19), we have the joint distribution $p(\boldsymbol{x}_{t+dt}^{-i}, \boldsymbol{x}_t^{-i})$ as

$$\begin{aligned}
& p(\boldsymbol{x}_{t+dt}^{-i}, \boldsymbol{x}_t^{-i}) \\
={}& \int dx_t^i p(\boldsymbol{x}_{t+dt}^{-i}|x_t^i, \boldsymbol{x}_t^{-i}) p(x_t^i, \boldsymbol{x}_t^{-i}) \\
={}& \frac{\mathcal{N}}{(2\pi)^{\frac{n_{\mathrm{sys}}}{2}} \sqrt{\det \Sigma_t}} \int d\bar{x}_t^i \exp\left[-\sum_{j'} \frac{dt}{4T_t^{j'}} (F_t^{j'} - \mu^{j'i}\bar{x}_t^i)^2 - \sum_{i'j'} \frac{1}{2} \bar{x}_t^{i'} G_t^{i'j'} \bar{x}_t^{j'} \right] \\
={}& \frac{\mathcal{N}}{(2\pi)^{\frac{n_{\mathrm{sys}}}{2}} \sqrt{\det \Sigma_t}} \exp\left[-\sum_{j'} \frac{dt}{4T_t^{j'}} (F_t^{j'})^2 - \sum_{i'j'} \frac{1}{2} \bar{x}_t^{i'} G_t^{i'j'} \bar{x}_t^{j'} \right] \\
& \times \sqrt{\frac{\pi}{\left(\sum_{j'} \frac{dt}{4T_t^{j'}} (\mu_t^{j'i})^2 + \frac{G_t^{ii}}{2} \right)}} \exp\left[\frac{\left[\sum_{j'} \left(G_t^{ij'} \bar{x}_t^{j'} - \frac{\mu_t^{j'i} F_t^{j'}}{2T_t^{j'}} dt \right) \right]^2}{4 \left(\sum_{j'} \frac{dt}{4T_t^{j'}} (\mu_t^{j'i})^2 + \frac{G_t^{ii}}{2} \right)} \right].
\end{aligned} \tag{8.20}$$

From Eqs. (8.18), (8.19) and (8.20), we obtain the analytical expression of the transfer entropy $dI_t^{\rm tr}$ up to the order of dt as

$$
\begin{aligned}
dI_t^{\rm tr} :=& \langle \ln p(\boldsymbol{x}_{t+dt}^{-i}|\boldsymbol{x}_t) + \ln p(\boldsymbol{x}_t^{-i}) - \ln p(\boldsymbol{x}_{t+dt}^{-i}, \boldsymbol{x}_t^{-i}) \rangle \\
=& \ln \mathcal{N} - \sum_{j'} \frac{dt}{4T_t^{j'}} \langle \left(F_t^{j'} - \mu_t^{j'i} \bar{x}_t^i \right)^2 \rangle - \frac{1}{2} \ln \left[(2\pi)^{n_{\rm sys}-1} (\det \tilde{\Sigma}_t) \right] - \sum_{i'j'} \frac{1}{2} \langle \bar{x}_t^{i'} \tilde{G}_t^{i'j'} \bar{x}_t^{j'} \rangle \\
& - \ln \mathcal{N} + \frac{1}{2} \ln [(2\pi)^{n_{\rm sys}} (\det \Sigma_t)] + \sum_{j'} \frac{dt}{4T_t^{j'}} \langle (F_t^{j'})^2 \rangle + \sum_{i'j'} \frac{1}{2} \langle \bar{x}_t^{i'} G_t^{i'j'} \bar{x}_t^{j'} \rangle \\
& - \frac{1}{2} \ln \pi + \frac{1}{2} \ln \left(\sum_{j'} \frac{dt}{4T_t^{j'}} (\mu_t^{j'i})^2 + \frac{G_t^{ii}}{2} \right) - \frac{\left\langle \left[\sum_{j'} \left(G_t^{ij'} \bar{x}_t^{j'} - \frac{\mu_t^{j'i} F_t^{j'}}{2T_t^{j'}} dt \right) \right]^2 \right\rangle}{4 \left(\sum_{j'} \frac{dt}{4T_t^{j'}} (\mu_t^{j'i})^2 + \frac{G_t^{ii}}{2} \right)} \\
=& \sum_{j'} \frac{(\mu_t^{j'i})^2 dt}{4G_t^{ii} T^{j'}} - \sum_{j'} \frac{dt}{4T_t^{j'}} (\mu_t^{j'i})^2 \Sigma_t^{ii} + \sum_{j'} \frac{\mu^{j'i} dt}{2T_t^{j'}} \langle F_t^{j'} \bar{x}_t^i \rangle - \sum_{i'} \frac{\delta_{i'i'}}{2} \\
& + \sum_{i'j'} \frac{\delta_{i'i'} - G_t^{i'i} \Sigma_t^{ii'}}{2} + \sum_{i'} \frac{G_t^{i'i} \Sigma_t^{ii'}}{2} \left(1 - \sum_{j'} \frac{dt}{2G_t^{ii} T_t^{j'}} (\mu_t^{j'i})^2 \right) \\
& + \sum_{i'j'} \frac{\mu_t^{j'i} dt}{2G_t^{ii} T_t^{j'}} G_t^{ii'} \langle F_t^{j'} \bar{x}_t^{i'} \rangle - \sum_{j'} \frac{(\mu_t^{j'i})^2 dt}{4G_t^{ii} T_t^{j'}} + \mathcal{O}(dt^2) \\
=& \sum_{j'} \frac{\mu^{j'i} dt}{2T_t^{j'}} \langle F_t^{j'} \bar{x}_t^i \rangle + \sum_{i'j'} \frac{\mu_t^{j'i} dt}{2G_t^{ii} T_t^{j'}} G_t^{ii'} \langle F_t^{j'} \bar{x}_t^{i'} \rangle - \sum_{j'} \frac{(\mu_t^{j'i})^2 dt}{4G_t^{ii} T_t^{j'}} + \mathcal{O}(dt^2) \\
=& \sum_{j'} \frac{(\mu_t^{j'i})^2}{4T_t^{j'}} \frac{\det \Sigma_t}{\det \tilde{\Sigma}_t} dt + \mathcal{O}(dt^2) \\
=& \frac{1}{2} \ln \left(1 + \sum_{j'} \frac{dP_t^{j'}}{N_t^{j'}} \right) + \mathcal{O}(dt^2),
\end{aligned}
\tag{8.21}
$$

where we define $dP_t^{j'} := [(\mu_t^{j'i})^2 \det \Sigma_t dt]/(\det \tilde{\Sigma}_t)$, and $N_t^{j'} := 2T_t^{j'}$, In this calculation, we used $G_t^{ii} = (\det \tilde{\Sigma}_t)/(\det \Sigma_t)$, $\sum_{j' \neq i} G_t^{i'j'} \Sigma_t^{j'l'} = \delta_{i'l'} - G_t^{i'i} \Sigma_t^{il'}$, $\langle F_t^{j'} \bar{x}_t^{i'} \rangle = \mu_t^{j'i} \Sigma_t^{ii'}$ and $\langle (F_t^{j'})^2 \rangle dt^2 = 2T^{j'} dt + \mathcal{O}(dt^2)$.

8.1.3 Relative Entropy and Integral Fluctuation Theorem for Small Subsystem

We show the integrated fluctuation theorems for a small subsystem which gives Eq. (8.14). Due to the detailed fluctuation theorem, $\Delta s_{\rm bath}^k$ is given by the ratio of the forward path probability and backward path probability such as

$$\Delta s^k_{\mathrm{bath}} := \ln \frac{p(x^i_{k+1}|x^i_k, \boldsymbol{x}^{-i}_k)}{p_B(x^i_k|x^i_{k+1}, \boldsymbol{x}^{-i}_{k+1})}, \tag{8.22}$$

where p_B is the backward path probability. Here we assume that the time interval between k and $k+1$ is infinitsimal. The conditional entropy production is given as

$$\sigma^{i|-i} = \ln \left[\frac{p(x^i_1|\boldsymbol{x}^{-i}_1)}{p(x^i_N|\boldsymbol{x}^{-i}_N)} \prod_{k=1}^{N-1} \frac{p(x^i_{k+1}|x^i_k, \boldsymbol{x}^{-i}_k)}{p_B(x^i_k|x^i_{k+1}, \boldsymbol{x}^{-i}_{k+1})} \right] \tag{8.23}$$

Let i^{tr}_k be the stochastic transfer entropy defined as $i^{\mathrm{tr}}_k := i(x^i_k : \boldsymbol{x}^{-i}_{k+1}|\boldsymbol{x}^{-i}_k)$, and i^{Btr}_k be the stochastic backward transfer entropy defined as $i^{\mathrm{Btr}}_k := i(x^i_{k+1} : \boldsymbol{x}^{-i}_k|\boldsymbol{x}^{-i}_{k+1})$. From Eqs. (8.2) and (8.22), we have

$$\sigma^{i|-i} - \sum_{k=1}^{N-1} i^{\mathrm{Btr}}_k + \sum_{k=1}^{N-1} i^{\mathrm{tr}}_k \tag{8.24}$$

$$= \ln \left[\frac{p(x^i_1|\boldsymbol{x}^{-i}_1)}{p(x^i_N|\boldsymbol{x}^{-i}_N)} \prod_{k=1}^{N-1} \frac{p(x^i_{k+1}|x^i_k, \boldsymbol{x}^{-i}_k)}{p_B(x^i_k|x^i_{k+1}, \boldsymbol{x}^{-i}_{k+1})} \frac{p(\boldsymbol{x}^{-i}_{k+1}|x^i_k, \boldsymbol{x}^{-i}_k)}{p(\boldsymbol{x}^{-i}_{k+1}|\boldsymbol{x}^{-i}_k)} \frac{p(\boldsymbol{x}^{-i}_k|\boldsymbol{x}^{-i}_{k+1})}{p(\boldsymbol{x}^{-i}_k|x^i_{k+1}, \boldsymbol{x}^{-i}_{k+1})} \right] \tag{8.25}$$

$$= \ln \left[\frac{p(x^i_1, \boldsymbol{x}^{-i}_1)}{p(x^i_N, \boldsymbol{x}^{-i}_N)} \prod_{k=1}^{N-1} \frac{p(x^i_{k+1}|x^i_k, \boldsymbol{x}^{-i}_k)}{p_B(x^i_k|x^i_{k+1}, \boldsymbol{x}^{-i}_{k+1})} \frac{p(\boldsymbol{x}^{-i}_{k+1}|x^i_k, \boldsymbol{x}^{-i}_k)}{p(\boldsymbol{x}^{-i}_k|x^i_{k+1}, \boldsymbol{x}^{-i}_{k+1})} \right] \tag{8.26}$$

$$= d_{\mathrm{KL}}(p(X^i, \boldsymbol{X}^{-i})||p_B(X^i, \boldsymbol{X}^{-i})), \tag{8.27}$$

$$p_B(X^i, \boldsymbol{X}^{-i}) := p(x^i_N, \boldsymbol{x}^{-i}_N) \prod_{k=1}^{N-1} p_B(x^i_k|x^i_{k+1}, \boldsymbol{x}^{-i}_{k+1}) p(\boldsymbol{x}^{-i}_k|x^i_{k+1}, \boldsymbol{x}^{-i}_{k+1}), \tag{8.28}$$

where we used the Bayes rule $p(\boldsymbol{x}^{-i}_{k+1}|\boldsymbol{x}^{-i}_k)p(\boldsymbol{x}^{-i}_k) = p(\boldsymbol{x}^{-i}_k|\boldsymbol{x}^{-i}_{k+1})p(\boldsymbol{x}^{-i}_k)$. $p_B(X^i, \boldsymbol{X}^{-i})$ satisfies the normalization of the probability such as

$$\sum_{X^i, \boldsymbol{X}^{-i}} p_B(X^i, \boldsymbol{X}^{-i})$$

$$:= \sum_{\{X^i, \boldsymbol{X}^{-i}\} \backslash \{x^i_1, \boldsymbol{x}^{-i}_1\}} p(x^i_N, \boldsymbol{x}^{-i}_N) \prod_{k=2}^{N-1} p_B(x^i_k|x^i_{k+1}, \boldsymbol{x}^{-i}_{k+1}) p(\boldsymbol{x}^{-i}_k|x^i_{k+1}, \boldsymbol{x}^{-i}_{k+1}) \tag{8.29}$$

$$= \cdots \tag{8.30}$$

$$= \sum_{\{x^i_N, \boldsymbol{x}^{-i}_N\}} p(x^i_N, \boldsymbol{x}^{-i}_N) \tag{8.31}$$

$$= 1. \tag{8.32}$$

From the nonnegativity of the stochastic relative entropy, we have Eq. (8.14):

$$\langle \sigma^{i|-i} \rangle - \sum_{k=1}^{N-1} I_k^{\mathrm{Btr}} + \sum_{k=1}^{N-1} I_k^{\mathrm{tr}} \geq 0, \tag{8.33}$$

with equality if and only if $p(X^i, \boldsymbol{X}^{-i}) = p_B(X^i, \boldsymbol{X}^{-i})$. The property $p(X^i, \boldsymbol{X}^{-i}) = p_B(X^i, \boldsymbol{X}^{-i})$ means that the local reversibility of a small subsystem X^i under the condition of the outside worlds $\boldsymbol{X}^{-i}$. From the identity Eq. (3.36), we can also prove the integrated fluctuation theorems corresponding to Eq. (8.14) as

$$\left\langle \exp\left[-\sigma^{i|-i} + \sum_{k=1}^{N-1} i_k^{\mathrm{Btr}} - \sum_{k=1}^{N-1} i_k^{\mathrm{tr}} \right] \right\rangle = 1. \tag{8.34}$$

We also show the integrated fluctuation theorem for a small subsystem which gives the weaker inequality $\langle \sigma^{i|-i} \rangle \geq -\sum_{k=1}^{N-1} I_k^{\mathrm{tr}}$. $\sigma^{i|-i} + \sum_{k=1}^{N-1} i_k^{\mathrm{tr}}$ can be rewritten by the stochastic relative entropy as

$$\sigma^{i|-i} + \sum_{k=1}^{N-1} i_k^{\mathrm{tr}} \tag{8.35}$$

$$= \ln \left[\frac{p(x_1^i|\boldsymbol{x}_1^{-i})}{p(x_N^i|\boldsymbol{x}_N^{-i})} \prod_{k=1}^{N-1} \frac{p(x_{k+1}^i|x_k^i, \boldsymbol{x}_k^{-i})}{p_B(x_k^i|x_{k+1}^i, \boldsymbol{x}_{k+1}^{-i})} \frac{p(\boldsymbol{x}_{k+1}^{-i}|x_k^i, \boldsymbol{x}_k^{-i})}{p(\boldsymbol{x}_{k+1}^{-i}|\boldsymbol{x}_k^{-i})} \right] \tag{8.36}$$

$$= d_{\mathrm{KL}}(p(X^i, \boldsymbol{X}^{-i})||p'_B(X^i, \boldsymbol{X}^{-i})), \tag{8.37}$$

$$p'_B(X^i, \boldsymbol{X}^{-i})) := p(x_N^i|\boldsymbol{x}_N^{-i}) p(\boldsymbol{x}_1^{-i}) \prod_{k=1}^{N-1} p_B(x_k^i|x_{k+1}^i, \boldsymbol{x}_{k+1}^{-i}) p(\boldsymbol{x}_{k+1}^{-i}|\boldsymbol{x}_k^{-i}), \tag{8.38}$$

where $p'_B(X^i, \boldsymbol{X}^{-i})$ satisfies the normalization of the probability as

$$\sum_{X^i, \boldsymbol{X}^{-i}} p'_B(X^i, \boldsymbol{X}^{-i}) := \sum_{\boldsymbol{X}^{-i}} p(\boldsymbol{x}_1^{-i}) \prod_{k=1}^{N-1} p(\boldsymbol{x}_{k+1}^{-i}|\boldsymbol{x}_k^{-i}) \tag{8.39}$$

$$= 1. \tag{8.40}$$

From the nonnegativity of the relative entropy and the identity Eq. (3.36), we have

$$\langle \sigma^{i|-i} \rangle \geq -\sum_{k=1}^{N-1} I_k^{\mathrm{tr}}, \tag{8.41}$$

$$\left\langle \exp\left[-\sigma^{i|-i} - \sum_{k=1}^{N-1} i_k^{\mathrm{tr}} \right] \right\rangle = 1. \tag{8.42}$$

8.1.4 Stochastic Energetics for Small Subsystem

From the energetic point of view, we can consider Eq. (8.15) as a relationship between work and free energy for a small subsystem X^i under the condition of other systems $\boldsymbol{X}^{-i}$. We here consider the particular case in which the temperature of each heat bath is uniform $T^i = 2/\beta$ and the initial state and final state are set in equilibrium. The probability distribution in initial and final state is given by

$$p_{\mathrm{eq}}(x^i, \boldsymbol{x}^{-i}) = Z^{-1} \exp[-\beta(H_S(x^i) + H_E(\boldsymbol{x}^{-i}) + H_I(x^i, \boldsymbol{x}^{-i}))], \tag{8.43}$$

where $H_S(x^i)$ is the Hamiltonian of the target system X^i, $H_E(\boldsymbol{x}^{-i})$ is the Hamiltonian of the other systems $\boldsymbol{X}^{-i}$, $H_I(x^i, \boldsymbol{x}^{-i})$ is the interaction Hamiltonian between them, and Z is the partition function:

$$Z = \int d\boldsymbol{x}^{-i} dx^i \exp[-\beta(H_S(x^i) + H_E(\boldsymbol{x}^{-i}) + H_I(x^i, \boldsymbol{x}^{-i}))]. \tag{8.44}$$

The conditional probability in initial and final state $p_{\mathrm{eq}}(x^i|\boldsymbol{x}^{-i})$ is given by

$$p_{\mathrm{eq}}(x^i|\boldsymbol{x}^{-i}) = p_{\mathrm{eq}}(\boldsymbol{x}^{-i})/[\int dx_i p_{\mathrm{eq}}(x^i, \boldsymbol{x}^{-i})] \tag{8.45}$$

$$= [Z^i(\boldsymbol{x}^{-i})]^{-1} \exp[-\beta H_{\mathrm{eff}}(x^i|\boldsymbol{x}^{-i})], \tag{8.46}$$

where we define the effective Hamiltonian in the system i as $H_{\mathrm{eff}}(x^i|\boldsymbol{x}^{-i}) := H_S(x^i) + H_I(x^i, \boldsymbol{x}^{-i})$. $Z^i(\boldsymbol{x}^{-i})$ is the partition function for the system X^i with fixed $\boldsymbol{X}^{-i}$: $Z_i(\boldsymbol{x}_{-i}) = \int dx_i \exp[-\beta H_{\mathrm{eff}}(x_i|\boldsymbol{x}_{-i})]$. Let effective free-energy be $\Delta F_{\mathrm{eff}}(\boldsymbol{x}^{-i}) := -\beta^{-1} \ln Z^i(\boldsymbol{x}^{-i}(\tau)) + \beta^{-1} \ln Z^i(\boldsymbol{x}^{-i}(0))$. We define the effective work as $W_{\mathrm{eff}}(x^i|\boldsymbol{x}^{-i}) := \sum_k \Delta s^k_{\mathrm{bath}} + H_{\mathrm{eff}}(x^i(\tau)|\boldsymbol{x}^{-i}(\tau)) - H_{\mathrm{eff}}(x^i(0)|\boldsymbol{x}^{-i}(0))$.

Then Eqs. (8.14) can be replaced by

$$\beta(\langle W_{\mathrm{eff}}(x^i|\boldsymbol{x}^{-i})\rangle - \langle \Delta F_{\mathrm{eff}}(\boldsymbol{x}^{-i})\rangle) \geq \int_0^\tau dt \frac{dI_t^{\mathrm{Btr}}}{dt} - \int_0^\tau dt \frac{dI_t^{\mathrm{tr}}}{dt} \tag{8.47}$$

$$\geq -\int_0^\tau dt \frac{dI_t^{\mathrm{tr}}}{dt}. \tag{8.48}$$

If the other systems $\boldsymbol{X}^{-i}$ are completely separated from the subsystem X^i, we have $H_I(x^i, \boldsymbol{x}^{-i}) = 0$, $\int_0^\tau dt[dI_t^{\mathrm{Btr}}/dt] = 0$ and $\int_0^\tau dt[dI_t^{\mathrm{tr}}/dt] = 0$. The definitions of the free energy and the work become the conventional ones which do not depend on the outside worlds $\mathbf{X}^{-i}$. Thus we can reproduce the conventional second law of thermodynamics, i.e., $\beta(\langle W\rangle - \Delta F) \geq 0$ from Eqs. (8.47).

8.2 Further Generalizations

We here discuss other expressions of information thermodynamic inequality, which are consistent with Eq. (8.14). We also show a generalization of information thermodynamics on causal networks, and importance of the backward transfer entropy.

8.2.1 Generalization for Fokker-Planck Equation

We here consider the following Langevin equation:

$$\begin{aligned} \dot{x}^i(t) &= f^i(x^1(t), \ldots, x^{n_{\rm sys}}(t)) + \xi^i(t), \\ \langle \xi^i(t)\xi^j(t')\rangle &= 2T^i_t \delta_{ij}\delta(t-t'), \\ \langle \xi^i(t)\rangle &= 0, \end{aligned} \tag{8.49}$$

with $i = 1, \ldots, n_{\rm sys}$, and the Fokker-Planck equation corresponding to the Langevin equation (8.49):

$$\partial_t p(x^i, \boldsymbol{x}^{-i}, t) = -\sum_i \partial_{x^i} j^{x^i}(x^i, \boldsymbol{x}^{-i}, t), \tag{8.50}$$

$$j^{x^i}(x^i, \boldsymbol{x}^{-i}, t) := f^i(x^i(t), \boldsymbol{x}^{-i}(t)) p(x^i, \boldsymbol{x}^{-i}, t) - T^i \partial_{x^i} p(x^i, \boldsymbol{x}^{-i}, t), \tag{8.51}$$

where $\boldsymbol{x}^{-i} := \{x^1, \ldots, x^{i-1}, x^{i+1}, \ldots, x^{n_{\rm sys}}\}$ denotes the dynamical variables of the other systems $\boldsymbol{X}^{-i}$. The mean local velocity for a small subsystem X^i is defined as

$$\nu^{x^i}(x^i, \boldsymbol{x}^{-i}, t) := \frac{j^{x^i}(x^i, \boldsymbol{x}^{-i}, t)}{p(x^i, \boldsymbol{x}^{-i}, t)} \tag{8.52}$$

$$= f^i(x^i(t), \boldsymbol{x}^{-i}(t)) - T^i \partial_{x^i} \ln p(x^i, \boldsymbol{x}^{-i}, t). \tag{8.53}$$

This mean local velocity gives the ensemble average of $\dot{x}^i$ under the condition of $(x^i, \boldsymbol{x}^{-i}, t)$ [74]. We here introduce a key quantity $\dot{s}^{x^i}(x^i, \boldsymbol{x}^{-i}, t)$ defined as

$$\dot{s}^{x^i}(x^i, \boldsymbol{x}^{-i}, t) \tag{8.54}$$

$$:= \frac{\dot{x}^i(t)\nu^{x^i}(x^i, \boldsymbol{x}^{-i}, t)}{T^i} \tag{8.55}$$

$$= \frac{1}{T^i}\dot{x}^i(t) f^i(x^i, \boldsymbol{x}^{-i}, t) - \dot{x}^i(t)\partial_{x^i} \ln p(x^i, \boldsymbol{x}^{-i}, t) \tag{8.56}$$

$$= \sigma^{x^i} - \dot{x}^i(t)\partial_{x^i} i(x^i : \boldsymbol{x}^{-i}; t), \tag{8.57}$$

where σ^{x^i} is the entropy production defined as

$$\sigma^{x^i} := \frac{1}{T^i}\dot{x}^i(t) f^i(x^i, \boldsymbol{x}^{-i}, t) - \dot{x}^i(t)\partial_{x^i} \ln p(x^i, t), \tag{8.58}$$

and $i(x^i : \boldsymbol{x}^{-i}; t)$ is the stochastic mutual information defined as

$$i(x^i : \boldsymbol{x}^{-i}; t) := \ln \frac{p(x^i, \boldsymbol{x}^{-i}, t)}{p(\boldsymbol{x}^{-i}, t) p(x^i, t)}. \tag{8.59}$$

We here show that the ensemble average of a key quantity $\dot{s}^{x^i}(x^i, \boldsymbol{x}^{-i}, t)$ is nonnegative,

$$\left\langle \dot{s}^{x^i}(x^i, \boldsymbol{x}^{-i}, t) \right\rangle = \left\langle \frac{\dot{x}^i(t)\nu^{x^i}(x^i, \boldsymbol{x}^{-i}, t)}{T^i} \right\rangle \tag{8.60}$$

$$= \left\langle \frac{[\nu^{x^i}(x^i, \boldsymbol{x}^{-i}, t)]^2}{T^i} \right\rangle \tag{8.61}$$

$$= \int dx^i d\boldsymbol{x}^{-i} \frac{[j^{x^i}(x^i, \boldsymbol{x}^{-i}, t)]^2}{T^i p(x^i, \boldsymbol{x}^{-i}, t)} \tag{8.62}$$

$$\geq 0, \tag{8.63}$$

with equality if and only if $j^{x^i}(x^i, \boldsymbol{x}^{-i}, t) = 0$. Thus we have an information thermodynamic inequality

$$\langle \sigma^{x^i} \rangle \geq \langle \dot{x}^i(t) \partial_{x^i} i(x^i : \boldsymbol{x}^{-i}; t) \rangle. \tag{8.64}$$

The inequality equivalent to Eq. (8.64) have been derived in several papers [129, 57, 56, 58]. This information thermodynamic inequality Eq. (8.64) corresponds to Eq. (8.10) in the infinitesimal time-interval limit:

$$S(x^i_{k+1}) - S(x^i_k) + \langle \Delta s^k_{\mathrm{bath}} \rangle \geq I(x^i_k : \{\boldsymbol{x}^{-i}_k, \boldsymbol{x}^{-i}_{k+1}\}) - I(x^i_{k+1} : \{\boldsymbol{x}^{-i}_k, \boldsymbol{x}^{-i}_{k+1}\}). \tag{8.65}$$

Using the Fokker-Planck expression Eq. (8.63), we here discuss a relationship between the conventional second law and information thermodynamic inequality. The sum of the ensemble averages of key quantities gives

$$\sum_i \langle \dot{s}^{x^i}(x^i, \boldsymbol{x}^{-i}, t) \rangle = \sum_i \frac{1}{T^i} \langle \dot{x}^i(t) f^i(x^i, \boldsymbol{x}^{-i}, t) \rangle - \frac{d}{dt} \langle \ln p(x^i, \boldsymbol{x}^{-i}, t) \rangle, \tag{8.66}$$

where we used $[d/dt] \ln p(x^i, \boldsymbol{x}^{-i}, t) = \sum_i \dot{x}^i(t) \partial_{x^i} \ln p(x^i, \boldsymbol{x}^{-i}, t)$. Thus, the sum of the ensemble averages of key quantities is equal to the ensemble average of the total entropy production. The second law of thermodynamics is given by

$$\sum_i \langle \dot{s}^{x^i}(x^i, \boldsymbol{x}^{-i}, t) \rangle \geq 0, \tag{8.67}$$

with equality if and only if $j^{x^i}(x^i, \boldsymbol{x}^{-i}, t) = 0$ for all i. The second law of thermodynamics always gives a weaker bound of the entropy production $\langle \sigma^{x^i} \rangle$ compared to the information thermodynamics, i.e.,

$$\langle \sigma^{x^i} \rangle \geq \langle \dot{x}^i(t) \partial_{x^i} i(x^i : \boldsymbol{x}^{-i}; t) \rangle \tag{8.68}$$

$$\geq \langle \dot{x}^i(t) \partial_{x^i} i(x^i : \boldsymbol{x}^{-i}; t) \rangle - \sum_{j \neq i} \langle \dot{s}^{x^j}(x^j, \boldsymbol{x}^{-j}, t) \rangle, \tag{8.69}$$

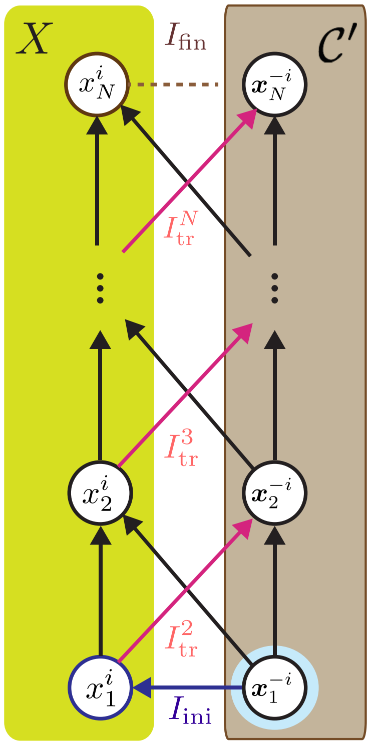

Fig. 8.2 A causal network corresponding to Eq. (8.70).

where Eq. (8.68) and Eq. (8.69) correspond to information thermodynamics and the conventional thermodynamics, respectively.

We stress that the term $\langle \dot{x}^i(t)\partial_{x^i} i(x^i : \boldsymbol{x}^{-i}; t)\rangle$ includes the contributions of both the transfer entropy and the backward transfer entropy in Eq. (8.10). If we did not consider the backward transfer entropy (e.g, Chapter 7), the bound of the entropy production $\langle \sigma^{x^i}\rangle$ given by the transfer entropy would not be always tighter than the bound given by the second law of thermodynamics.

8.2.2 Backward Transfer Entropy and Final Correlation

We here discuss the importance of the backward transfer entropy in the study of information thermodynamics on causal networks. We first consider the following dynamics

$$p(X^i, \boldsymbol{X}^{-i}) = p(x^i_1, \boldsymbol{x}^{-i}_1) \prod_{k=1}^{N-1} p(x^i_{k+1}|x^i_k, \boldsymbol{x}^{-i}_k) p(\boldsymbol{x}^{-i}_{k+1}|x^i_k, \boldsymbol{x}^{-i}_k). \tag{8.70}$$

We can consider a causal network for Eq. (8.70) (see Fig. 8.2). This causal network shows multi-time steps of the Markovian dynamics from time 1 to time N. By the discussion in Chapter 6, the entropy production for a small subsystem X^i is bounded by the information quantity Θ, which is given by the graph Fig. 8.2 as

$$\Theta := i_{\mathrm{fin}} - i_{\mathrm{ini}} - \sum_{l=1}^{N} i_{\mathrm{tr}}^{l}, \tag{8.71}$$

$$\begin{aligned} i_{\mathrm{ini}} &= i(x_1 : \mathrm{pa}(x_1)) \\ &= i(x_1^i : \boldsymbol{x}_1^{-i}), \end{aligned} \tag{8.72}$$

$$\begin{aligned} i_{\mathrm{tr}}^{1} &= i(c_1 : \mathrm{pa}_X(c_1)) \\ &= 0, \end{aligned} \tag{8.73}$$

$$\begin{aligned} i_{\mathrm{tr}}^{l} &= i(c_l : \mathrm{pa}_X(c_l)|c_l) \quad [2 \le l \le N] \\ &= i(x_{l-1}^i : \boldsymbol{x}_l^{-i}|\boldsymbol{x}_{l-1}^{-i}, \dots, \boldsymbol{x}_1^{-i}), \end{aligned} \tag{8.74}$$

$$\begin{aligned} i_{\mathrm{fin}} &= i(x^2 : \mathcal{C}') \\ &= i(x_N^i : \{\boldsymbol{x}_N^{-i}, \dots, \boldsymbol{x}_1^{-i}\}), \end{aligned} \tag{8.75}$$

where we set $X = \{x_1 = x_1^i, \dots, x_N = x_N^i\}$, $\mathcal{C} = \mathcal{C}' = \{c_1 = \boldsymbol{x}_1^{-i}, \dots, c_N = \boldsymbol{x}_N^{-i}\}$, $\mathrm{pa}(x_1^i) = \boldsymbol{x}_1^{-i}$, $\mathrm{pa}_X(\boldsymbol{x}_1^{-i}) = \emptyset$, and $\mathrm{pa}_X(\boldsymbol{x}_l^{-i}) = x_{l-1}^i$ with $2 \le l \le N$. Thus, the information thermodynamic inequality Eq. (6.41) gives

$$\langle \sigma \rangle \ge \langle \Theta \rangle \tag{8.76}$$

$$= I(x_N^i : \{\boldsymbol{x}_N^{-i}, \dots, \boldsymbol{x}_1^{-i}\}) - I(x_1^i : \boldsymbol{x}_1^{-i}) - \sum_{l=2}^{N} I(x_{l-1}^i : \boldsymbol{x}_l^{-i}|\boldsymbol{x}_{l-1}^{-i}, \dots, \boldsymbol{x}_1^{-i}) \tag{8.77}$$

$$\begin{aligned} =& I(x_N^i : \boldsymbol{x}_N^{-i}) - I(x_1^i : \boldsymbol{x}_1^{-i}) \\ &+ \sum_{l=2}^{N} I(x_N^i : \boldsymbol{x}_{l-1}^{-i}|\boldsymbol{x}_l^{-i}, \dots, \boldsymbol{x}_N^{-i}) - \sum_{l=2}^{N} I(x_{l-1}^i : \boldsymbol{x}_l^{-i}|\boldsymbol{x}_{l-1}^{-i}, \dots, \boldsymbol{x}_1^{-i}). \end{aligned} \tag{8.78}$$

On the other hand, the causal network for the single time step [see Figure 8.1)] gives another information thermodynamic inequality which corresponds to Eq. (8.14):

$$\langle \sigma \rangle \ge I(x_N^i : \boldsymbol{x}_N^{-i}) - I(x_1^i : \boldsymbol{x}_1^{-i}) + \sum_{l=2}^{N} I(x_l^i : \boldsymbol{x}_{l-1}^{-i}|\boldsymbol{x}_l^{-i}) - \sum_{l=2}^{N} I(x_{l-1}^i : \boldsymbol{x}_l^{-i}|\boldsymbol{x}_{l-1}^{-i}) \tag{8.79}$$

$$\begin{aligned} =& I(x_N^i : \boldsymbol{x}_N^{-i}) - I(x_1^i : \boldsymbol{x}_1^{-i}) \\ &+ \sum_{l=2}^{N} I(x_l^i : \boldsymbol{x}_{l-1}^{-i}|\boldsymbol{x}_l^{-i}, \dots, \boldsymbol{x}_N^{-i}) - \sum_{l=2}^{N} I(x_{l-1}^i : \boldsymbol{x}_l^{-i}|\boldsymbol{x}_{l-1}^{-i}, \dots, \boldsymbol{x}_1^{-i}), \end{aligned} \tag{8.80}$$

where we used $p(\boldsymbol{x}_l^{-i}|x_{l-1}^i, \boldsymbol{x}_{l-1}^{-i}) = p(\boldsymbol{x}_l^{-i}|x_{l-1}^i, \boldsymbol{x}_{l-1}^{-i}, \dots, \boldsymbol{x}_1^{-i})$ and $p(\boldsymbol{x}_{l-1}^{-i}|x_l^i, \boldsymbol{x}_l^{-i}) = p(\boldsymbol{x}_{l-1}^{-i}|x_l^i, \boldsymbol{x}_l^{-i}, \dots, \boldsymbol{x}_N^{-i})$.

Here we have the following conditional Markov property:

$$\begin{aligned} & p(x_N^i, x_l^i, \boldsymbol{x}_{l-1}^{-i}|\boldsymbol{x}_l^{-i}, \dots, \boldsymbol{x}_N^{-i}) \\ &= p(\boldsymbol{x}_{l-1}^{-i}|\boldsymbol{x}_l^{-i}, \dots, \boldsymbol{x}_N^{-i}) p(x_l^i|\boldsymbol{x}_{l-1}^{-i}, \boldsymbol{x}_l^{-i}, \dots, \boldsymbol{x}_N^{-i}) p(x_N^i|x_l^i, \boldsymbol{x}_l^{-i}, \dots, \boldsymbol{x}_N^{-i}). \end{aligned} \tag{8.81}$$

Then we have $I(x^i_N : \boldsymbol{x}^{-i}_{l-1} | x^i_l, \boldsymbol{x}^{-i}_l, \dots, \boldsymbol{x}^{-i}_N) = 0$ and the following data processing inequality:

$$I(x^i_N : \boldsymbol{x}^{-i}_{l-1} | \boldsymbol{x}^{-i}_l, \dots, \boldsymbol{x}^{-i}_N) \leq I(x^i_l : \boldsymbol{x}^{-i}_{l-1} | \boldsymbol{x}^{-i}_l, \dots, \boldsymbol{x}^{-i}_N) + I(x^i_N : \boldsymbol{x}^{-i}_{l-1} | x^i_l, \boldsymbol{x}^{-i}_l, \dots, \boldsymbol{x}^{-i}_N) \tag{8.82}$$

$$= I(x^i_l : \boldsymbol{x}^{-i}_{l-1} | \boldsymbol{x}^{-i}_l, \dots, \boldsymbol{x}^{-i}_N). \tag{8.83}$$

Thus the difference between two information bounds is nonnegative, and we have

$$\langle \sigma \rangle \geq I(x^i_N : \boldsymbol{x}^{-i}_N) - I(x^i_1 : \boldsymbol{x}^{-i}_1) + \sum_{l=2}^{N} I(x^i_l : \boldsymbol{x}^{-i}_{l-1} | \boldsymbol{x}^{-i}_l) - \sum_{l=2}^{N} I(x^i_{l-1} : \boldsymbol{x}^{-i}_l | \boldsymbol{x}^{-i}_{l-1}) \tag{8.84}$$

$$\geq I(x^i_N : \{\boldsymbol{x}^{-i}_N, \dots, \boldsymbol{x}^{-i}_1\}) - I(x^i_1 : \boldsymbol{x}^{-i}_1) - \sum_{l=2}^{N} I(x^i_{l-1} : \boldsymbol{x}^{-i}_l | \boldsymbol{x}^{-i}_{l-1}, \dots, \boldsymbol{x}^{-i}_1). \tag{8.85}$$

This calculation indicates that the sum of information thermodynamic inequalities for the single time step [e.g., Eq. (8.80)] gives a tighter bound of the entropy production rather than the multi-time steps (e.g., Eq. (8.78)). This fact suggests a possibility of further generalization of information thermodynamics on causal networks using the backward transfer entropy instead of the final correlation $I_{\rm fin}$.

8.2.3 Further Generalization: Information Thermodynamics on Causal Networks Including Backward Transfer Entropy

We here consider the replacement of the final correlation $I_{\rm fin}$ by the backward transfer entropy in the study of information thermodynamics on causal networks in Chapter 6. Let N'' be the number of elements of $\mathcal{C}'$ [i.e., $\mathcal{C}' = \{c_1, \dots, c_{N''}\}$]. The final correlation is calculated as

$$I_{\rm fin} = I(x_N : \mathcal{C}') \tag{8.86}$$

$$= I(x_N : c_{N''}) + \sum_{l=1}^{N''-1} I(x_N : c_l | c_{l+1}, \dots, c_{N''}). \tag{8.87}$$

We here define the set of children of c_l, $\mathrm{ch}(c_l) := \{a_k | c_l \in \mathrm{pa}(a_k)\}$. Let $\mathrm{ch}_X(c_l)$ be the intersection of X and $\mathrm{ch}(c_l)$, i.e., $\mathrm{ch}_X(c_l) := \mathrm{ch}(c_l) \cap X$. Here we define the set $\mathcal{D}_l$ as

$$\mathcal{D}_l := \bigcup_{l'=1}^{l} \mathrm{ch}_X(c_{l'}). \tag{8.88}$$

Because $\mathcal{D}_l$ is the subset of X [i.e., $\mathcal{D}_l \subseteq X$], we can uniquely define

$$x_{\rm sup}(c_l) := x_k, \tag{8.89}$$

which satisfies $k \geq k'$ for all $x_{k'} \in \mathcal{D}_l$. In the case of $\mathcal{D}_l = \emptyset$, $x_{\sup}(c_l)$ is given by $x_{\sup}(c_l) := \emptyset$. The variable $x_{\sup}(c_l)$ denotes the latest state of X, where the history of the other systems $\{c_1, \ldots, c_l\}$ can affect as a child.

Here we have the following conditional Markov properties:

$$\begin{aligned} &p(c_l, x_{\sup}(c_l), x_N | c_{l+1}, \ldots, c_{N''}) \\ &= p(c_l | c_{l+1}, \ldots, c_{N''}) p(x_{\sup}(c_l) | c_l, c_{l+1}, \ldots, c_{N''}) p(x_N | x_{\sup}(c_l), c_{l+1}, \ldots, c_{N''}), \end{aligned} \tag{8.90}$$

and

$$\begin{aligned} &p(c_{N''}, x_{\sup}(c_{N''}), x_N) \\ &= p(c_{N''}) p(x_{\sup}(c_{N''}) | (c_{N''})) p(x_N | x_{\sup}(c_{N''})). \end{aligned} \tag{8.91}$$

Then we have $I(c_l : x_N | x_{\sup}(c_l), c_{l+1}, \ldots, c_{N''}) = 0$, $I(c_{N''} : x_N | x_{\sup}(c_{N''})) = 0$ and the following data processing inequalities:

$$\begin{aligned} I(x_N : c_l | c_{l+1}, \ldots, c_{N''}) &\leq I(x_{\sup}(c_l) : c_l | c_{l+1}, \ldots, c_{N''}), \\ I(x_N : c_{N''}) &\leq I(x_{\sup}(c_{N''}) : c_{N''}). \end{aligned} \tag{8.92}$$

We define the backward transfer entropy on causal network as

$$I^l_{\mathrm{Btr}} := I(x_{\sup}(c_l) : c_l | c_{l+1}, \ldots, c_{N''}), \tag{8.93}$$

$$I^{N''}_{\mathrm{Btr}} := I(x_{\sup}(c_{N''}) : c_{N''}), \tag{8.94}$$

with $1 \leq l \leq N''-1$. From the data processing inequalities (8.92), the finial correlation I_{fin} is smaller than the sum of the backward transfer entropy I^l_{Btr},

$$I_{\mathrm{fin}} \leq \sum_{l=1}^{N''} I^l_{\mathrm{Btr}}, \tag{8.95}$$

with equality if $x_{\sup}(c_l) = x_N$ for all l.

We here show that new informational quantity $\sum_{l=1}^{N''} I^l_{\mathrm{Btr}} - I_{\mathrm{ini}} - \sum_{l=1}^{N''} I^l_{\mathrm{tr}}$ gives a lower bound of the ensemble average of the entropy production $\langle \sigma \rangle$. Let i^l_{Btr} be the stochastic backward transfer entropy on causal network defined as

$$i^l_{\mathrm{Btr}} := i(x_{\sup}(c_l) : c_l | c_{l+1}, \ldots, c_{N''}), \tag{8.96}$$

$$i^{N''}_{\mathrm{Btr}} := i(x_{\sup}(c_{N''}) : c_{N''}), \tag{8.97}$$

with $1 \leq l \leq N'' - 1$. We define an informational quantity Θ' corresponding to $\sum_{l=1}^{N''} I^l_{\mathrm{Btr}} - I_{\mathrm{ini}} - \sum_{l=1}^{N''} I^l_{\mathrm{tr}}$ as

$$\Theta' := \sum_{l=1}^{N''} i^l_{\mathrm{Btr}} - i_{\mathrm{ini}} - \sum_{l=1}^{N''} i^l_{\mathrm{tr}}. \tag{8.98}$$

We show that the difference between the entropy production and the informational quantity $\sigma - \Theta'$ can also be rewritten as the stochastic relative entropy:

$$
\begin{aligned}
&\sigma - \Theta' \\
=& \ln \left[\frac{p(x_1)}{p(x_N)} \prod_{k=1}^{N-1} \frac{p(x_{k+1}|x_k, \mathcal{B}_{k+1})}{p_B(x_k|x_{k+1}, \mathcal{B}_{k+1})} \right] + \ln \frac{p(x_1|\mathrm{pa}(x_1))}{p(x_1)} - \ln \frac{p(c_{N''}|x_{\mathrm{sup}}(c_l))}{p(c_{N''})} \\
&- \sum_{l=1}^{N''-1} \ln \frac{p(c_l|x_{\mathrm{sup}}(c_l), c_{l+1}, \dots, c_{N''})}{p(c_l|c_{l+1}, \dots, c_{N''})} + \sum_{l|c_l \in \mathcal{C}'} \ln \frac{p(c_l|\mathrm{pa}(c_l))}{p(c_l|c_{l-1}, \dots, c_1)} \\
=& \ln \left[\prod_{k=1}^{N} p(x_k|\mathrm{pa}(x_k)) \prod_{l|c_l \in \mathcal{C}'} p(c_l|\mathrm{pa}(c_l)) \right] \\
&- \ln \left[\prod_{k=1}^{N-1} p_B(x_k|x_{k+1}, \mathcal{B}_{k+1}) p(x_N) \prod_{l=1}^{N''} p(c_l|x_{\mathrm{sup}}(c_l), c_{l+1}, \dots, c_{N''}) \right] \\
=& d_{\mathrm{KL}}(p(\mathcal{V})||p'_B(\mathcal{V})),
\end{aligned}
\tag{8.99}
$$

where $p(c_l|x_{\mathrm{sup}}(c_l), c_{l+1}, \dots, c_{N''})|_{l=N''} = p(c_l|x_{\mathrm{sup}}(c_l))$, and we define the new backward path probability $p'_B(\mathcal{V})$ as

$$
\begin{aligned}
&p'_B(\mathcal{V}) \\
:=& \prod_{k=1}^{N-1} p_B(x_k|x_{k+1}, \mathcal{B}_{k+1}) p(x_N) \prod_{l=1}^{N''} p(c_l|x_{\mathrm{sup}}(c_l), c_{l+1}, \dots, c_{N''}) \prod_{l'|c_{l'} \notin \mathcal{C}'} p(c_{l'}|\mathrm{pa}(c_{l'})).
\end{aligned}
\tag{8.100}
$$

We here define the set $\mathcal{C}'(x_k)$ as $\mathcal{C}'(x_k) := \{c_l \in \mathcal{C}' | x_{\mathrm{sup}}(c_l) = x_k\}$. We have $\mathcal{C}'(x_k) \cap \mathcal{B}_{k+1} = \emptyset$. Thus the backward path probability satisfies the normalization of the probability as

$$\sum_{\mathcal{V}} p'_B(\mathcal{V}) \tag{8.101}$$

$$= \sum_{X,\mathcal{C}'} \left[\prod_{k=1}^{N-1} p_B(x_k|x_{k+1}, \mathcal{B}_{k+1}) p(x_N) \prod_{c_l \in \mathcal{C}'} p(c_l|x_{\sup}(c_l), c_{l+1}, \dots, c_{N''}) \right] \tag{8.102}$$

$$= \sum_{X,\{\mathcal{C}' \setminus \mathcal{C}'(x_1)\}} \left[\prod_{k=1}^{N-1} p_B(x_k|x_{k+1}, \mathcal{B}_{k+1}) p(x_N) \right.$$

$$\left. \times \prod_{\{c_l \in \mathcal{C}', c_l \notin \mathcal{C}'(x_1)\}} p(c_l|x_{\sup}(c_l), c_{l+1}, \dots, c_{N''}) \right] \tag{8.103}$$

$$= \sum_{\{X \setminus x_1\},\{\mathcal{C} \setminus \mathcal{C}'(x_1)\}} \left[\prod_{k=2}^{N-1} p_B(x_k|x_{k+1}, \mathcal{B}_{k+1}) p(x_N) \right.$$

$$\left. \times \prod_{\{c_l \in \mathcal{C}', c_l \notin \mathcal{C}'(x_1)\}} p(c_l|x_{\sup}(c_l), c_{l+1}, \dots, c_{N''}) \right] \tag{8.104}$$

$$= \cdots$$

$$= \sum_{x_N, \{c_l \in \mathcal{C}'(x_N)\}} \left[p(x_N) \prod_{\{c_l \in \mathcal{C}'(x_N)\}} p(c_l|x_{\sup}(c_l), c_{l+1}, \dots, c_{N''}) \right]$$

$$= \sum_{x_N} p(x_N) \tag{8.105}$$

$$= 1. \tag{8.106}$$

This new backward path probability $p'_B(\mathcal{V})$ indicates that we consider the backward path probability only for the target system X (i.e., $p_B(x_k|x_{k+1}, \mathcal{B}_{k+1})$) under the condition of other system $\mathcal{C}$ (i.e., $\prod_{\{c_l \in \mathcal{C}'(x_k)\}} p(c_l|x_{\sup}(c_l), c_{l+1}, \dots, c_{N''})$) "for each time step k", where the probability distribution of $\mathcal{C}$ is given by the distribution of the forward process $p(\mathcal{V})$. This new backward path probability $p'_B(\mathcal{V})$ is given by multiplication of conditional probabilities for each time step k, while $p_B(\mathcal{V})$ in Chap. 6 (i.e., Eq.(6.37)) is given by the backward path probability for a whole time evolution from x_1 to x_N.

From the identity Eq. (3.36) and the nonnegativity of the stochastic relative entropy $D_{\mathrm{KL}}(p(\mathcal{V})||p'_B(\mathcal{V})) \geq 0$, we have the generalizations of the integral fluctuation theorem and the second law of thermodynamics,

$$\langle \exp[-\sigma + \Theta'] \rangle = 1, \tag{8.107}$$

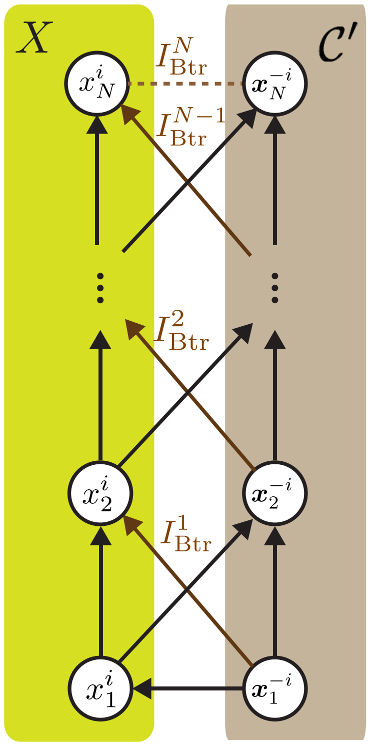

Fig. 8.3 Example of the backward transfer entropy on causal network corresponding to Eq. (8.70).

$$\langle \sigma \rangle \geq \sum_{l=1}^{N''} I_{\mathrm{Btr}}^l - I_{\mathrm{ini}} - \sum_{l=1}^{N''} I_{\mathrm{tr}}^l \tag{8.108}$$

$$\geq I_{\mathrm{fin}} - I_{\mathrm{ini}} - \sum_{l=1}^{N''} I_{\mathrm{tr}}^l, \tag{8.109}$$

where we used Eq. (8.95).

8.2.4 Examples of Generalized Second Law Including Backward Transfer Entropy

Finally, we apply this generalization Eq. (8.108) to the causal networks corresponding to multi-time steps of the Markovian dynamics Eq. (8.70), and the complex dynamics in multiple fluctuating systems discussed in Chapter 6 previously. The backward transfer entropy gives tighter bounds of the entropy production for these two causal networks.

8.2.4.1 Example 1: Mulit-time steps of the Markovian dynamics

We here consider the causal networks in Figure 8.3, which represents the multi-time steps of the Markovian dynamics from time 1 to N. The information quantity Θ' is calculated as

$$\Theta' := \sum_{l=1}^{N} i_{\mathrm{Btr}}^{l} - i_{\mathrm{ini}} - \sum_{l=1}^{N} i_{\mathrm{tr}}^{l}, \tag{8.110}$$

$$\begin{aligned} i_{\mathrm{ini}} &= i(x_1 : \mathrm{pa}(x_1)) \\ &= i(x_1^i : \boldsymbol{x}_1^{-i}), \end{aligned} \tag{8.111}$$

$$\begin{aligned} i_{\mathrm{tr}}^{1} &= i(c_1 : \mathrm{pa}_X(c_1)) \\ &= 0, \end{aligned} \tag{8.112}$$

$$\begin{aligned} i_{\mathrm{tr}}^{l} &= i(c_l : \mathrm{pa}_X(c_l)|c_l) \quad [2 \leq l \leq N] \\ &= i(x_{l-1}^i : \boldsymbol{x}_l^{-i}|\boldsymbol{x}_{l-1}^{-i}, \ldots, \boldsymbol{x}_1^{-i}), \end{aligned} \tag{8.113}$$

$$\begin{aligned} i_{\mathrm{Btr}}^{l} &= i(x_{\mathrm{sup}}(c_l) : c_l|c_{l+1}, \ldots, c_{N''}) \quad [1 \leq l \leq N-1] \\ &= i(x_{l+1}^i : \boldsymbol{x}_l^{-i}|\boldsymbol{x}_{l+1}^{-i}, \ldots, \boldsymbol{x}_N^{-i}), \\ i_{\mathrm{Btr}}^{N} &= i(x_{\mathrm{sup}}(c_N) : c_N) \\ &= i(x_N^i : \boldsymbol{x}_N^{-i}), \end{aligned} \tag{8.114}$$

where we set $X = \{x_1 = x_1^i, \ldots, x_N = x_N^i\}$, $\mathcal{C} = \mathcal{C}' = \{c_1 = \boldsymbol{x}_1^{-i}, \ldots, c_N = \boldsymbol{x}_N^{-i}\}$, $\mathrm{pa}(x_1^i) = \boldsymbol{x}_1^{-i}$, $\mathrm{pa}_X(\boldsymbol{x}_1^{-i}) = \emptyset$, $\mathrm{pa}_X(\boldsymbol{x}_l^{-i}) = x_{l-1}^i$ with $2 \leq l \leq N$, $x_{\mathrm{sup}}(\boldsymbol{x}_l^{-i}) = x_{l+1}^i$ with $1 \leq l \leq N-1$, and $x_{\mathrm{sup}}(\boldsymbol{x}_N^{-i}) = x_N^i$. Thus, the information thermodynamic inequality including the backward transfer entropy Eq. (8.108) gives the following inequality, which is equivalent to Eq. (8.80):

$$\langle \sigma \rangle \geq \langle \Theta' \rangle \tag{8.115}$$

$$\begin{aligned} &= I(x_N^i : \boldsymbol{x}_N^{-i}) - I(x_1^i : \boldsymbol{x}_1^{-i}) \\ &\quad + \sum_{l=2}^{N} I(x_l^i : \boldsymbol{x}_{l-1}^{-i}|\boldsymbol{x}_l^{-i}, \ldots, \boldsymbol{x}_N^{-i}) - \sum_{l=2}^{N} I(x_{l-1}^i : \boldsymbol{x}_l^{-i}|\boldsymbol{x}_{l-1}^{-i}, \ldots, \boldsymbol{x}_1^{-i}). \end{aligned} \tag{8.116}$$

8.2.4.2 Example 2: Complex dynamics

We next consider the causal networks in Figure 8.4 which represents the complex dynamics in multiple fluctuating systems. The information quantity Θ' is calculated as

$$\Theta' := \sum_{l=1}^{N} i_{\mathrm{Btr}}^{l} - i_{\mathrm{ini}} - \sum_{l=1}^{N} i_{\mathrm{tr}}^{l}, \tag{8.117}$$

$$\begin{aligned} i_{\mathrm{ini}} &= i(x_1 : \mathrm{pa}(x_1)) \\ &= i(x_1 : y_1), \end{aligned} \tag{8.118}$$

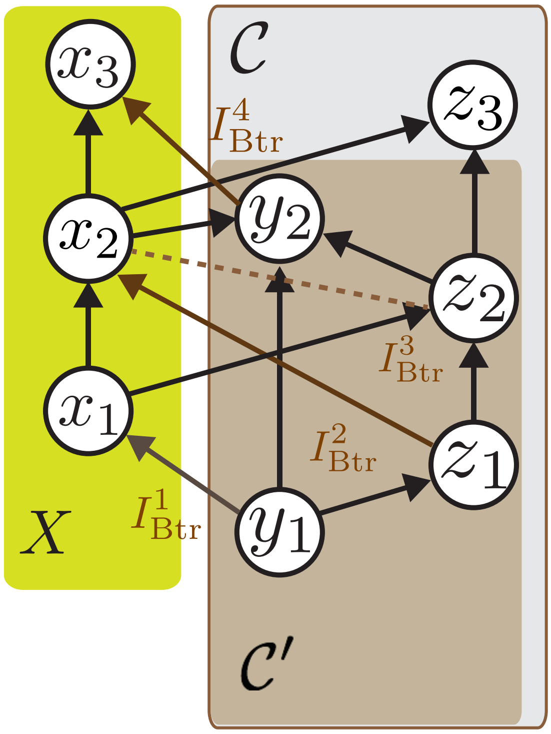

Fig. 8.4 Example of the backward transfer entropy on causal network of the complex dynamics.

$$
\begin{aligned}
i^1_{\rm tr} &= i(c_1 : {\rm pa}_X(c_1)) \\
&= 0, && (8.119) \\
i^2_{\rm tr} &= i(c_2 : {\rm pa}_X(c_2)|c_1) \\
&= 0, && (8.120) \\
i^3_{\rm tr} &= i(c_3 : {\rm pa}_X(c_3)|c_2, c_1) \\
&= i(z_2 : x_1|z_1, y_1), && (8.121) \\
i^4_{\rm tr} &= i(c_4 : {\rm pa}_X(c_4)|c_3, c_2, c_1) \\
&= i(y_2 : x_2|y_1, z_1, z_2), && (8.122)
\end{aligned}
$$

$$
\begin{aligned}
i^1_{\rm Btr} &= i(x_{\rm sup}(c_1) : c_1|c_2, c_3, c_4) \\
&= i(x_1 : y_1|z_1, z_2, y_2), && (8.123) \\
i^2_{\rm Btr} &= i(x_{\rm sup}(c_2) : c_2|c_3, c_4) \\
&= i(x_2 : z_1|z_2, y_2), && (8.124) \\
i^3_{\rm Btr} &= i(x_{\rm sup}(c_3) : c_3|c_4) \\
&= i(x_2 : z_2|y_2), && (8.125) \\
i^4_{\rm Btr} &= i(x_{\rm sup}(c_4) : c_4) \\
&= i(x_3 : y_2), && (8.126)
\end{aligned}
$$

where we set $X = \{x_1, x_2, x_3\}$, $\mathcal{C} = \{c_1 = y_1, c_2 = z_1, c_3 = z_2, c_4 = y_2, c_5 = z_3\}$, $\mathcal{C}' = \{c_1, \ldots, c_4\}$, $\mathrm{pa}(x_1) = y_1$, $\mathrm{pa}_X(y_1) = \emptyset$, $\mathrm{pa}_X(z_1) = \emptyset$, $\mathrm{pa}_X(z_2) = x_1$, $\mathrm{pa}_X(y_2) = x_2$, $x_{\mathrm{sup}}(y_1) = x^1$, $x_{\mathrm{sup}}(z_1) = x^2$, $x_{\mathrm{sup}}(z_2) = x^2$, and $x_{\mathrm{sup}}(y_2) = x^3$. Thus, the information thermodynamic inequality including the backward transfer entropy Eq. (8.108) gives the following inequality:

$$\langle \sigma \rangle \geq \langle \Theta' \rangle \tag{8.127}$$

$$= I(x_{\mathrm{sup}}(c_4) : c_4) + I(x_2 : z_2 | y_2) + I(x_2 : z_1 | z_2, y_2) + I(x_1 : y_1 | z_1, z_2, y_2)$$
$$- I(x_1 : y_1) - I(z_2 : x_1 | z_1, y_1) - I(y_2 : x_2 | y_1, z_1, z_2). \tag{8.128}$$

Chapter 9

Further applications

In this chapter, we show several applications of information thermodynamics on causal networks such as the steady-state thermodynamics (see also Sec. 3.2.1 and 3.2.2) and the feedback cooling (see also Sec. 3.2.3). We first discuss an applications to the steady-state thermodynamics for coupled Langevin equations. The definition of the entropy production on causal network Eq. (6.9) is given by the ratio of the forward path probability and backward path probability. To replace the definition of the backward path probability, i.e., $p_B(x_k|x_{k+1}, \mathcal{B}_{k+1})$, with the (backward) path probability of the dual dynamics Eq. (3.57) (Eq. (3.63)) as in the steady-state thermodynamics, we can easily show the relationship between the housekeeping heat (excess heat) and information. We next discuss an application to the feedback cooling. By applying our main result (6.41) to the coupled underdamped Langevin equation, we discuss the cooling bound and the third law of thermodynamics from a view point of information flow. Our discussion based on the information thermodynamic inequality is different from the discussion of the paper given by K. H. Kim and H. Qian [116] (i.e., Eq. (3.75)).

9.1 Steady State Information Thermodynamics

Here, we generalize the steady-state thermodynamics in terms of information transfer. We consider the following two dimensional Langevin system:

$$\begin{aligned}
\gamma_x \dot{x}(t) &= f^x_{\rm ex}(x, y, \lambda(t)) - \partial_x U(x, y, \lambda(t)) + \xi^x_t, \\
\gamma_y \dot{y}(t) &= f^y_{\rm ex}(x, y, \lambda(t)) - \partial_y U(x, y, \lambda(t)) + \xi^y_t, \\
\langle \xi^x(t) \rangle &= 0, \\
\langle \xi^x(t) \xi^{x'}(t') \rangle &= 2\gamma_x T^x \delta_{xx'} \delta(t - t'),
\end{aligned} \tag{9.1}$$

where $f^x_{\rm ex}$ ($f^y_{\rm ex}$) is an external nonconservative force, and $\lambda(t)$ is the control parameter. We here define the nonequilibrium potential $\phi(x, y, \lambda)$ as

$$\phi(x, y, \lambda) = -\ln p_{\rm ss}(x, y; \lambda), \tag{9.2}$$

where $p_{\rm ss}(x, y; \lambda)$ is the steady-state distribution corresponding to a control parameter λ. The mean local velocity of the nonequilibrium steady state in X is defined as

$$\gamma_x v^x_{\rm ss}(x, y, \lambda) = f^x_{\rm ex}(x, y, \lambda) - \partial_x U(x, y, \lambda) + T^x \partial_x \phi(x, y, \lambda). \tag{9.3}$$

We consider the path $\mathbf{x} = \{x_1, \dots, x_N\}$, where $x_k := x(kdt)$, $y_k := y(kdt)$ and $\lambda_k := \lambda(kdt)$ with an infinitesimal time interval dt. The conditional probability of the Langevin dynamics Eq. (3.42) is given by

$$p(x_{k+1}|x_k, y_k) = \mathcal{N}_x \exp\left[-\frac{(\gamma_x x_{k+1} - \gamma_x x_k - f^x_{\rm tot}(x_k, y_k, \lambda_k)dt)^2}{4\gamma^x T^x dt} \right]. \tag{9.4}$$

where $f^x_{\rm tot}(x, y, \lambda) := f^x_{\rm ex}(x, y, \lambda) - \partial_x U(x, y, \lambda)$ denotes the total force in X. Here, we introduce the dual dynamics in X. The conditional probability of the dual dynamics $p_D(x_{k+1}|x_k, y_k)$ is given by

$$\begin{aligned} &p_D(x_{k+1}|x_k, y_k) \\ &= \mathcal{N}_x \exp\left[-\frac{(\gamma_x x_{k+1} - \gamma_x x_k - f_{\rm tot}(x_k, y_k, \lambda_k)dt + 2\gamma_x v^x_{\rm ss}(x_k, y_k, \lambda_k)dt)^2}{4\gamma_x T^x dt} \right]. \end{aligned} \tag{9.5}$$

Up to the order $o(dt)$, the stochastic relative entropy $d_{\rm KL}(p(x_{k+1}, x_k, y_k)||p_D(x_{k+1}, x_k, y_k))$ is calculated as

$$\begin{aligned} &d_{\rm KL}(p(x_{k+1}, x_k, y_k)||p_D(x_{k+1}, x_k, y_k)) \\ &= \frac{1}{T^x}(x_{k+1} - x_k)\frac{\gamma_x v^x_{\rm ss}(x_k, y_k, \lambda_k) + \gamma_x v^x_{\rm ss}(x_{k+1}, y_{k+1}\lambda_{k+1})}{2} &(9.6) \\ &= \frac{1}{T^x} Q^x_{\rm hk}(kdt), &(9.7) \end{aligned}$$

where the housekeeping heat $Q^x_{\rm hk}(t)$ in X at time t is defined as

$$Q^x_{\rm hk}(t) := [\dot{x}(t) \circ \gamma_x v^x_{\rm ss}(x(t), y(t), \lambda(t))]dt. \tag{9.8}$$

From the nonnegativity of the relative entropy $D_{\rm KL}(p(x_{k+1}, x_k, y_k)||p_D(x_{k+1}, x_k, y_k)) \geq 0$, we have

$$\langle Q^x_{\rm hk}(t) \rangle \geq 0. \tag{9.9}$$

This housekeeping heat inequality is a generalization of the information thermodynamic inequality for two-dimensional Langevin system, because Eq. (9.9) is equivalent to the information thermodynamic inequality Eq. (8.65) if we replace the steady state distribution $p_{\rm ss}(x, y, \lambda)$ by the conventional probablility distribution $p(x(t), y(t))$.

We can also derive another generalization of the information thermodynamics for a steady state. The backward probability of the dual dynamics $p_{BD}(x_k|x_{k+1}, y_k)$ is given by

$$
\begin{aligned}
&p_{BD}(x_k|x_{k+1}, y_{k+1}) \\
&= \mathcal{N}_x \exp\left[-\frac{(\gamma_x(x_k - x_{k+1}) + f^x_{\mathrm{tot}}(x_{k+1}, y_{k+1}, \lambda_{k+1})dt + 2T^x \partial_x \phi(x_{k+1}, y_{k+1}, \lambda_{k+1})dt)^2}{4\gamma_x T^x dt} \right].
\end{aligned}
\tag{9.10}
$$

We here define $p_{BD}(x_k, x_{k+1}, y_k, y_{k+1})$ as

$$
p_{BD}(x_k, x_{k+1}, y_k, y_{k+1}) := p_{BD}(x_k|x_{k+1}, y_{k+1}) p(x_{k+1}, y_k, y_{k+1}). \tag{9.11}
$$

Up to the order $o(dt)$, the stochastic relative entropy between p and p_{BD} is calculated as

$$
\begin{aligned}
&d_{\mathrm{KL}}(p(x_k, x_{k+1}, y_k, y_{k+1}) || p_{BD}(x_k, x_{k+1}, y_k, y_{k+1})) \\
&= \ln p(x_k) - \ln p(x_{k+1}) + (x_{k+1} - x_k) \frac{\partial_x \phi(x_k, y_k, \lambda_k) + \partial_x \phi(x_{k+1}, y_{k+1}, \lambda_{k+1})}{2} \\
&+ i(x_k : \{y_k, y_{k+1}\}) - i(x_{k+1} : \{y_k, y_{k+1}\}) \\
&= \ln p(x_k) - \ln p(x_{k+1}) + \frac{1}{T^x} Q^x_{\mathrm{ex}}(kdt) + i(x_k : \{y_k, y_{k+1}\}) - i(x_{k+1} : \{y_k, y_{k+1}\}),
\end{aligned}
\tag{9.12}
$$

where $Q^x_{\mathrm{ex}}(t)$ is the excess heat in X at time t defined as

$$
Q^x_{\mathrm{ex}}(t) := -\frac{dt}{T^x} \dot{x}(t) \circ \partial_x \phi(x(t).y(t), \lambda(t)). \tag{9.13}
$$

From the nonnegativity of the relative entropy, we have another generalization of the steady state thermodynamics with information

$$
\Delta s_x + \frac{1}{T^x} \langle Q^x_{\mathrm{ex}}(kdt) \rangle \geq I(x_{k+1} : \{y_k, y_{k+1}\}) - I(x_k : \{y_k, y_{k+1}\}), \tag{9.14}
$$

where the Shannon entropy difference is defined as $\Delta s_x := \langle \ln p(x_k) \rangle - \langle \ln p(x_{k+1}) \rangle$, which can be replaced by the nonequilibrium potential change if $p(x_k)$ and $p(x_{k+1})$ are steady state distributions. This inequality implies that the information flow term $I(x_{k+1} : \{y_k, y_{k+1}\}) - I(x_k : \{y_k, y_{k+1}\})$ is important if we consider the steady state thermodynamics for coupled dynamics.

9.2 Feedback Cooling and Third Law of Thermodynamics

Next, we discuss the relationship between feedback cooling and information thermodynamics. By applying the information thermodynamic inequality (6.61) to the coupled underdamped Langevin equation, we discuss a cooling bound of the kinetic (effective) temperature and the information flow. This result is a generalization of our previous discussion of feedback cooling with information [31].

We here consider the following coupled underdamped Langevin equation, which describes the feedback cooling:

$$m\ddot{x}(t) = -\gamma[\dot{x}(t) - y(t)] + \xi^x(t), \tag{9.15}$$

$$\dot{y}(t) = -\frac{1}{\tau^y}[y(t) - \dot{x}(t)] + \xi^y(t), \tag{9.16}$$

$$\langle \xi^x(t) \rangle = \langle \xi^y(t) \rangle = 0, \tag{9.17}$$

$$\langle \xi^x(t)\xi^x(t') \rangle = 2\gamma T^x(t)\delta(t-t'), \tag{9.18}$$

$$\langle \xi^y(t)\xi^y(t') \rangle = 2\frac{T^y(t)}{\tau^y}\delta(t-t'), \tag{9.19}$$

$$\langle \xi^x(t)\xi^y(t') \rangle = 0, \tag{9.20}$$

where y denotes the memory state of the spontaneous velocity $\dot{x}$, $\tau^y > 0$ is a time constant which corresponds to the operation time intervals of the feedback controller, m is the mass of the particle, and γ is the friction constant.

The heat absorption in X [72, 74] is given by

$$J^x(t) := \langle \dot{x}(t) \circ [\xi^x(t) - \gamma\dot{x}(t)] \rangle \tag{9.21}$$

$$= \frac{\gamma}{m}[T^x(t) - \langle m\dot{x}^2(t) \rangle], \tag{9.22}$$

where we used the relation of the Startonovich integral $\langle \dot{x}(t) \circ \xi^x(t) \rangle = \gamma T^x(t)/m$. From the information thermodynamic inequality (7.8), we have

$$\frac{J^x(t)}{T^x(t)}dt \leq dI_t^{\mathrm{tr}} - dI_t^{\mathrm{Btr}} - dS_t^{x|y} \tag{9.23}$$

$$\leq dI_t^{\mathrm{tr}} - dS_t^{x|y}, \tag{9.24}$$

where the transfer entropy is defined as $dI_t^{\mathrm{tr}} := \langle \ln p(y(t+dt)|\dot{x}(t), y(t)) - \ln p(y(t+dt)|y(t)) \rangle$, the backward transfer entropy is defined as $dI_t^{\mathrm{Btr}} := \langle \ln p(y(t)|\dot{x}(t+dt), y(t+dt)) - \ln p(y(t)|y(t+dt)) \rangle$, and the conditional Shannon entropy is given by $dS_t^{x|y} := \langle \ln p(\dot{x}(t)|y(t)) - \ln p(\dot{x}(t+dt)|y(t+dt)) \rangle$. In a stationary state, the conditional Shannon entropy vanishes, i.e., $dS_t^{x|y} = 0$, and the information thermodynamic inequality (9.24) can be rewritten as

$$\frac{T^x(t) - T_{\mathrm{eff}}(t)}{T^x(t)}\frac{dt}{t_r} \leq dI_t^{\mathrm{tr}} - dI_t^{\mathrm{Btr}} \tag{9.25}$$

$$\leq dI_t^{\mathrm{tr}}, \tag{9.26}$$

where $T_{\mathrm{eff}}(t) := \langle m\dot{x}^2(t) \rangle$ is the kinetic temperature and $t_r := m/\gamma > 0$ is the relaxation time. This inequality gives a lower bound of the kinetic temperature $T_{\mathrm{eff}}(t)$ from a viewpoint of the transfer entropy dI_t^{tr}.

We here assume that the probability distribution is a Gaussian distribution with $\langle \dot{x}(t) \rangle = \langle y(t) \rangle = 0$. From the analytical calculation in Chapter 7, we analytically obtained the transfer entropy dI_t^{tr} as

$$dI_t^{\mathrm{tr}} = \frac{1}{2}\ln\left(1 + \frac{1-(\rho_t^{xy})^2}{\tau^y}\frac{\langle \dot{x}^2(t)\rangle dt}{2T^y(t)}\right) \tag{9.27}$$

$$= \frac{1-(\rho_t^{xy})^2}{4\tau^y}\frac{T_{\mathrm{eff}}(t)dt}{T^y(t)}, \tag{9.28}$$

where $(\rho_t^{xy}) := [\langle \dot{x}(t)y(t)\rangle^2]/[\langle \dot{x}^2(t)\rangle\langle y^2(t)\rangle]$ is a correlation coefficient which satisfies $(\rho_t^{xy})^2 \leq 1$. Thus, the inequality (9.26) gives

$$\frac{T^x(t) - T_{\mathrm{eff}}(t)}{T^x(t)}\frac{dt}{t_r} \leq \frac{1}{4\tau^y}\frac{T_{\mathrm{eff}}(t)dt}{T^y(t)}, \tag{9.29}$$

or

$$T^x(t)\left[\frac{t_r}{4\tau^y}\frac{T^x(t)}{T^y(t)} + 1\right]^{-1} \leq T_{\mathrm{eff}}(t). \tag{9.30}$$

This inequality indicates that the kinetic temperature $T_{\mathrm{eff}}(t)$ can be lower than the temperature of the heat bath $T^x(t)$ because of the feedback control effect. The lower bound of the kinetic temperature cannot be zero, if the time constant τ^y is finite. This fact is related to the third law of thermodynamics, which states that it is impossible for any process, no matter how idealized, to reduce the entropy of a system to its absolute zero value in a finite number of operations. [123].

We add that another statement of the third law of thermodynamics is generally proved from the property of the transfer entropy at the zero temperature. In the case where the system X is in a stationary state at the absolute zero temperature, the probability distributions of X are given by the delta functions, i.e., $p(\dot{x}(t)) = \delta(\dot{x}(t))$ and $p(\dot{x}(t)|y(t)) = \delta(\dot{x}(t))$. The conditional Shannon entropy vanishes [i.e., $dS_t^{x|y} = 0$], and the transfer entropy dI_t^{tr} is calculated as

$$dI_t^{\mathrm{tr}} = \int dy(t+dt)dy(t)d\dot{x}(t)\left[p(y(t+dt), y(t)|\dot{x}(t))p(\dot{x}(t))\ln\frac{p(y(t+dt)|y(t), \dot{x}(t))}{p(y(t+dt)|y(t))}\right] \tag{9.31}$$

$$= \int dy(t+dt)dy(t)\left[p(y(t+dt), y(t)|\dot{x}(t)=0)\ln\frac{p(y(t+dt)|y(t), \dot{x}(t)=0)}{p(y(t+dt)|y(t), \dot{x}(t)=0)}\right] \tag{9.32}$$

$$= 0. \tag{9.33}$$

Thus, the information thermodynamic inequality (9.24) gives

$$\Delta s_{\mathrm{bath}} := -\frac{J^x(t)}{T^x(t)}dt \geq 0, \tag{9.34}$$

which implies that the entropy change Δs_{bath} associated with any other systems cannot be reduced as the temperature approaches absolute zero. This is another statement of the third law of thermodynamics [123].

Chapter 10

Conclusions

We have studied thermodynamics with complex information flows induced by interactions between multiple fluctuating systems. The main results are in Chapters 6, 7, 8, and 9. We here summarize our results in this thesis and discuss an influence of our study, a scope of application, our future prospects.

In Chapter 6, we have developed stochastic thermodynamics for multiple fluctuating systems based on the causal networks. To divide nodes of the casual networks into two parts, the target system and the other systems, we have discussed thermodynamics for a small subsystem under the condition of the other systems [50]. We have defined thermodynamical quantities and informational quantities using the terminologies of the directed acyclic graph, (i.e., the set of parents and the topology ordering). One of the main results is a novel generalization of the second law for a small subsystems on causal networks. In this study, we have used the causal networks as the tool for deriving the novel generalization of the second law of thermodynamics. We believe that our formalism is well established because concepts of the causality, the transfer entropy, and the second law of thermodynamics are closely related to each other. We also add that this study would be important because thermodynamics is well formulated on causal networks. It can be a future challenge to apply several technique of the Bayesian networks, such as the machine learning and pattern recognition, to the nonequilibrium thermodynamics.

We also believe that the technique in our study can be used for several studies of causal networks. The informational quantity $\langle \Theta \rangle$ may have a meaning even if we do not discuss thermodynamics, but discuss the other fields of study on causal networks (e.g., the financial marketing described by causal networks). The informational quantity $\langle \Theta \rangle$ can be calculated in a realistic situation described by causal networks, because $\langle \Theta \rangle$ is the measurable quantity given by the mutual information and the conditional mutual information.

In Chapter 7, we have discussed the biochemical signal transduction using the main result in Chapter 6 as a simple application of our studysystems [59]. We have showed that the transfer entropy gives the lower bound of the robustness of the biochemical signal transduction with a feedback loop. In our discussion, we have only focused on the simple dynamics of sensory adaptation described by the coupled Langevin equation. From the discussion in Chapter 6, we can discuss the accuracy of any signal transduction which has a complex structure and a time-delay effect. In general, the robustness of the signal transduction is bounded by the informational quantity $\langle \Theta \rangle$, which can be calculated from the topology of signal transduction networks. In the case of the complex biochemical signal transduction, we can use the technique of causal networks to treat numerous experimental data.

We have also discuss thermodynamic efficiency of information transmission in terms of thermodynamics. Our study may answer the question how to determine the biochemical parameter (e.g., time constant) in a real biological cell. In the process of the evolution, it is not so strange that the biochemical system may obtain the efficient parameter, and such a biochemical parameter may be optimized to maximize information-thermodynamic efficiency as a total thermodynamic system.

In Chapter 8, we have discussed the further generalization of the study in Chapter 6. Applying the data processing inequality, we have showed that the backward transfer entropy, which is the novel information flow that we proposed, give a tighter bound of the entropy production. In our generalization, the backward transfer entropy can be considered as the inevitable loss of thermodynamic benefit. We believe that the importance in the study of Chapter 8 is the proposal of the backward transfer entropy as a loss of benefit. We believe that the backward transfer entropy can be an important measure of causal relationship between two time series likewise the conventional transfer entropy. It is interesting that the relationship between the backward transfer entropy and several applications of the conventional transfer entropy such as the Granger causality [106, 107], the phase-transition [128], and the time series analysis [105, 108, 109].

In Chapter 9, we have shown the possibilities of the application of our study. Several nonequilibrium dynamics, such as the steady-state thermodynamics and the feedback cooling, can be discussed using our formalism of information thermodynamics. We believe that information flow, i.e., the transfer entropy and the backward transfer entropy, can be an important quantity in nonequilibrium statistical physics in many situations. We believe that several nonequilibrium dynamics of multiple fluctuating system can be discussed quantitatively characterizing the information flow. For example, we have showed that the information thermodynamics gives the cooling bound by information for a feedback cooling system.

We here note an influence of our research in terms of a list of citations from our two papers [50, 59], which include the main topic of this thesis. Our research have led to several studies of the generalized second law of thermodynamics for a subsystem in a class of Markov process [56, 57, 58, 168] and in a class of non-Markovian process [169, 170], several studies of a relationship between thermodynamics and information in a biochemical sensory system [60, 62, 63], several studies of thermodynamics with information processing [61, 167, 171, 172, 173, 174, 175, 176] and other topics of thermodynamics [177, 178, 179].

We add a limit of application of our study. Our main result Eq. (6.41) (or Eq. (8.108)) is the relationship between the entropy production σ and the informational quantity Θ (or Θ'). We discuss a limit of application of our study in terms of the validity of these two definitions. First, the informational quantity is based on a classical stochastic process with causality, therefore our main result is not directly applicable to quantum dynamics. This fact does not mean an inability of a generalization of our study for quantum dynamics, because thermodynamics with information processing can be discussed for quantum dynamics in a simple setup (e.g., Ref. [167]). Second, the definition of the entropy production σ is based on the definition of the detailed fluctuation theorem [70, 72, 74], therefore it depends on the definition of the backward path probability p_B. As discussed in Chap. 9, the definition of the backward path probability can be replaced, and the physical meaning of σ can be changed, while maintaining the information thermodynamic inequality (6.41). This fact suggests that we have to take care of choice of p_B in each case, to obtain a meaningful (thermodynamic) quantity σ. For example, in the case of a Langevin equation with a colored noise, it is difficult to define the backward path probability p_B and an instantaneous value of the entropy change in the heat baths. We add that the assumption Eq. (6.2) is not satisfied in the case of a Langevin equation with a colored noise.

In our result, we have developed stochastic thermodynamics for a small subsystem interacting with fluctuating multiple other systems, and discussed the robustness of the biochemical signal transduction. Our theory can provide a physical basis of nonequilibrium dynamics with information and bioinformatics as Shannon's information theory for artificial communication. Our study has a potential to apply to not only several nonequilibrium dynamics, but also information dynamics on causal networks.

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